Although ECHA is providing a lot of online material in your language, part of this page is only in English. More about ECHA's multilingual practice.

Close **Do not show this message again**

Please be aware that this old REACH registration data factsheet is no longer maintained; it remains frozen as of 19th May 2023.

The new ECHA CHEM database has been released by ECHA, and it now contains all REACH registration data. There are more details on the transition of ECHA's published data to ECHA CHEM <u>here</u>.

Access ECHA CHEM

Use of this information is subject to copyright laws and may require the permission of the owner of the information, as described in the ECHA Legal Notice.

REACH

N,N,N',N'-tetramethylhexamethylenediamine

EC number: 203-842-9 CAS number: 111-18-2

JK

Environmental fate & pathways
Bioaccumulation: aquatic / sediment

001 Weight of evidence | (Q)SAR

Administrative data

Endpoint:	bioaccumulation in aquatic species: fish					
Type of information:	(Q)SAR					
Adequacy of study:	weight of evidence					
Reliability:	2 (reliable with restrictions)					
Rationale for reliability incl. deficiencies:	results derived from a valid (Q)SAR model and falling into its applicability domain, with adequate and reliable documentation / justification					
Remarks:	Based on the mean absolute errors of the models the confidence in the predicted results is high.					
Justification for type of information:	1. SOFTWARE T.E.S.T. (version 4.2.1) (Toxicity Estimation Software Tool). US EPA, 2012.					
	2. MODEL (incl. version number) T.E.S.T. (version 4.2.1); BCF model					
	3. SMILES OR OTHER IDENTIFIERS USED AS INPUT FOR THE MODEL See section 'Test Material'.					
	4. SCIENTIFIC VALIDITY OF THE (Q)SAR MODEL See attached QMRF.					
	5. APPLICABILITY DOMAIN See attached QPRF.					
	 6. ADEQUACY OF THE RESULT The model is scientifically valid (see attached QMRF). The model estimates the bioconcentration factor (BCF) as required information point under Regulation (EC) No 1907/2006 [REACH], Annex IX, 9.3.2 Bioaccumulation in aquatic species, preferably fish (see also attached QPRF). See attached QPRF for reliability assessment. 					

Data source

Reference 1 Reference Type: other: BCF calculation Title: Unnamed

Year:	2016
Report date:	2016

Reference 2

Reference Type:	other: Estimation software
Title:	T.E.S.T. (Toxicity Estimation Software Tool), v4.2.1
Author:	US EPA
Year:	2016
Bibliographic source:	United States Environmental Protection Agency, Washington, DC, USA

Materials and methods

Principles of method if other T.E.S.T. is a toxicity estimation software tool. The program than guideline: requires only the molecular structure of the test item, all other molecular descriptors which are required to estimate the toxicity are calculated within the tool itself. The molecular descriptors describe physical characteristics of the molecule (e.g. E-state values and E-state counts, constitutional descriptors, topological descriptors, walk and path counts, connectivity, information content, 2d autocorrelation, Burden eigenvalue, molecular property (such as the octanol-water partition coefficient), Kappa, hydrogen bond acceptor/donor counts, molecular distance edge, and molecular fragment counts). Each of the available methods uses a different set of these descriptors to estimate the toxicity. The bioaccumulation factor (BCF) was estimated using several available methods: hierarchical clustering method; FDA method, single model method; group contribution method; nearest neighbor method; consensus method. The methods were validated using statistical external validation using separate training and test data sets. The experimental data set was obtained from several different databases (Dimitrov et al., 2005; Arnot and Gobas, 2006; EURAS; Zhao, 2008). From the available data set salts, mixtures and ambiguous compounds were removed. The final data set contained 676 chemicals. References: - Dimitrov, S., N. Dimitrova, T. Parkerton, M. Combers, M. Bonnell, and O. Mekenyan. 2005. Base-line model for identifying the bioaccumulation potential of chemicals. SAR and QSAR in Environmental Research 16:531-554. - Arnot, J.A., and F.A.P.C. Gobas. 2006. A review of bioconcentration factor (BCF) and bioaccumulation factor (BAF) assessments for organic chemicals in aquatic organisms. Environ. Rev. 14:257-297. - EURAS. Establishing a bioconcentration factor (BCF) Gold Standard Database. EURAS [cited 5/20/09]. Available from http://www.euras.be/eng/project.asp?ProjectId=92. - Zhao, C.; Boriani, E.; Chana, A.; Roncaglioni, A.; Benfenati, E. 2008. A new hybrid system of QSAR models for predicting bioconcentration factors (BCF). Chemosphere 73:1701-1707.

GLP compliance:

no

Test material

Test material	information					
Constituent 1						
	Reference substance name:	N,N,N',N'-tetramethylhexamethylenediamine				
-NN	EC Number:	203-842-9				
	EC Name:	N,N,N',N'-tetramethylhexamethylenediamine				
	Cas Number:	111-18-2				
	Molecular formula:	C10H24N2				
	IUPAC Name:	[6-(dimethylamino)hexyl]dimethylamine				
Test material form:	liquid					

Test organisms

Test organisms (species): other: fish

Test conditions

Details on estimation of bioconcentration:	BASIS FOR CALCULATION OF BCF - Estimation software: US EPA T.E.S.T. v4.2.1
	Applied estimation methods:
	- Hierarchical clustering
	- FDA
	- Single model
	- Group contribution
	- Nearest neighbor
	- Consensus

Results and discussion

Bioaccumulation fa	ctor
Туре:	BCF
Value:	9.92 L/kg
Remarks on result:	other: method: consensus (average of reasonable results from all models); log BCF = 1.0; Based on the mean absolute error, the confidence in the predicted BCF values is high.

Any other information on results incl. tables

Model details:

Method	Predicted value		Model statistics			MAE (in log10)			
						External test set		Training set	
	log BCF	BCF	r²	q²	No. of chemicals	Entire set	SC >= 0.5	Entire set	SC >= 0.5
Consensus method	1.00	9.92	-	-	-	0.51	0.38	0.42	0.42
Hierarchical clustering	1.12	13.09 (8.57- 20.00)	0.748 - 0.981	0.669 - 0.970	12 - 540 (cluster models: 10)	0.54	0.91	0.23	0.14
Single model	1.16	14.59 (1.09- 195.81)	0.764	0.733	540	0.54	0.48	0.53	0.53
Group contribution	1.33	21.40 (0.68- 669.33)	0.719	0.527	499	0.62	0.56	0.60	0.83
FDA	-0.44	0.36 (0.05- 2.39)	0.909	0.840	29	0.57	0.64	0.53	0.68
Nearest neighbor	1.81	65.3	-	-	3	0.60	0.51	0.55	0.38

Legend:

MAE = mean absolute error

SC = similarity coefficient

r² = correlation coefficient

q² = leave one out correlation coefficient

Applicant's summary and conclusion

Information on Registered Substances comes from registration dossiers which have been assigned a registration number. The assignment of a registration number does however not guarantee that the information in the dossier is correct or that the dossier is compliant with Regulation (EC) No 1907/2006 (the REACH Regulation). This information has not been reviewed or verified by the Agency or any other authority. The content is subject to change without prior notice.



Reproduction or further distribution of this information may be subject to copyright protection. Use of the information without obtaining the permission from the owner(s) of the respective information might violate the rights of the owner.