Lamotrigine

Other names:	1,2,4-Triazine-3,5-diamine, 6-(2,3-dichlorophenyl)-
	3,5-Diamino-6-(2,3-dichlorophenyl)-1,2,4-triazine
	3,5-Diamino-6-(2,3-dichlorophenyl)-as-triazine
	6-(2,3-Dichlorophenyl)-1,2,4-triazine-3,5-diamine
	BW 430C
	LTG
	Lamictal
Inchi:	InChI=1S/C9H7Cl2N5/c10-5-3-1-2-4(6(5)11)7-8(12)14-9(13)16-15-7/h1-3H,(H4,12,13,14
InchiKey:	PYZRQGJRPPTADH-UHFFFAOYSA-N
Formula:	C9H7Cl2N5
SMILES:	N=c1nnc(-c2cccc(Cl)c2Cl)c(N)[nH]1
Mol. weight [g/mol]:	256.09
CAS:	84057-84-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Aqueous Solubility Prediction Method
logp	1.358		Crippen Method
mcvol	164.530	ml/mol	McGowan Method

Sources

Experimental determination and correlation of lamotrigine solubility in aqueous mixtures of 1-octyl-3-methylimidazolium chloride ionic liquid at various temperatures:	https://www.doi.org/10.1016/j.jct.2019.03.024
Lamotrigine Solubility in Some Nonaqueous Solvent Mixtures at 298.2 K:	https://www.doi.org/10.1021/acs.jced.5b00355
Solubility of Lamotrigine, Diazepam, and Clonazepam in Ethanol + Water Mixtures at 298.15 K:	https://www.doi.org/10.1021/je8007827
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The effect of 1-hexyl-3-methylimidazolium bromide ionic liquid as a co-solvent on the solubility of lamotrigine at T = 293.2–313.2 K:	https://www.doi.org/10.1016/j.jct.2019.02.013
Solubility of Clonazepam, Diazepam, Lamotrigine, and Phenobarbital in Propylene Glycol + Water Mixtures at 298.15 K:	https://www.doi.org/10.1021/je9000153
Solubility of Lamotrigine, Diazepam, Clonazepam, and Phenobarbital in Methanol + Water Mixtures at 298.2 K:	https://www.doi.org/10.1021/je800931z
Measurement and Thermodynamic Modeling of the Solubility of Lamotrigine, Deferiprone, Cefixime Trihydrate, and Cephalexin Monohydrate in Different Pure Solvents from 283.1 to 323.1 K:	https://www.doi.org/10.1021/acs.jced.6b00163
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84057841&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

https://www.chemeo.com/cid/98-867-2/Lamotrigine.pdf

Generated by Cheméo on 2025-12-05 18:11:48.915821639 +0000 UTC m=+4706506.445862303.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.