

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

Measurement and Thermodynamic Modeling of the Solubility of Lamotrigine, Diazepam, Clonazepam, Lamotrigine, and Phenobarbital in Aqueous and Propylene Glycol + Water Mixtures at 298.2 K: Monohydrate in Different Pure Solvents from 283.1 to 323.1 K: McGowan Method.

<https://www.doi.org/10.1021/acs.jced.6b00163>

<https://www.doi.org/10.1021/acs.jced.5b00355>

The effect of 1-hexyl-3-methylimidazolium bromide ionic liquids as co-solvent on the solubility of lamotrigine, diazepam, clonazepam, and phenobarbital in aqueous mixtures of ethanol + water at 298.15 K: Crippen Method.

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

<http://link.springer.com/article/10.1007/BF02311772>

<https://www.doi.org/10.1016/j.jct.2019.02.013>

<https://www.doi.org/10.1021/je9000153>

<https://www.doi.org/10.1016/j.jct.2019.03.024>

<https://www.doi.org/10.1021/je8007827>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C84057841&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Solubility of Lamotrigine, Diazepam, Clonazepam, and Phenobarbital in Propylene Glycol + Water Mixtures at 298.15 K:

<https://www.doi.org/10.1021/je800931z>

Legend

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

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