Carbamazepine

Other names:	5-Carbamoyl-5H-Dibenz[b,f]azepine
	5-Carbamoyl-5H-dibenzo(b,f)azepine
	5-Carbamoyldibenzo(b,f)azepine
	5-Carbamyl-5H-dibenzo(b,f)azepine
	5-Carbamyldibenzo(b,f)azepine
	5-Carbomoyl-5H-dibenzo(b,f)azepine
	5H-Dibenz[b,f]azepine-5-carboxamide
	5H-Dibenz[b,f]azepine-5-carboxamine
	5H-dibenz[b,f]azepine-5-carboxamide (carbamazepine)
	Amizepin
	Biston
	Calepsin
	Carbamazepen
	Carbamezepine
	Carbatrol
	Carbazepine
	Carbelan
	Epitol
	Equetro
	Finlepsin
	G 32883
	Geigy 32883
	Iminostilbene-N-carboxamide
	Karbamazepin
	Lexin
	NSC 169864
	Neurotol
	Sirtal
	Stazepin
	Stazepine
	Tegretal
	Tegretol
	Telesmin
	Timonil
Inchi:	InChI=1S/C15H12N2O/c16-15(18)17-13-7-3-1-5-11(13)9-10-12-6-2-4-8-14(12)17/h1-10H
InchiKey:	FFGPTBGBLSHEPO-UHFFFAOYSA-N
Formula:	C15H12N2O
SMILES:	NC(=O)N1c2ccccc2C=Cc2ccccc21
Mol. weight [g/mol]:	236.27
CAS:	298-46-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Aqueous Solubility Prediction Method
log10ws	-3.29		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	3.387		Crippen Method
mcvol	181.060	ml/mol	McGowan Method
rinpol	2270.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2337.00		NIST Webbook
rinpol	2285.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2397.40		NIST Webbook
rinpol	2296.00		NIST Webbook
rinpol	2259.00		NIST Webbook
rinpol	2259.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2290.00		NIST Webbook
tf	466.15	K	Solubility of Carbamazepine (Form III) in Different Solvents from (275 to 343) K
tf	463.74	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	25.60	kJ/mol	465.30	NIST Webbook

Sources

Solubility of Carbamazepine (Form III) in Different Solvents from (275 to 343) K:	https://www.doi.org/10.1021/je8002157
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C298464&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility Determination for Carbamazepine and Saccharin in Methanol/Water Mixed Solvent: Basic Data for Design of Cocrystal Production by Antisolvent Crystallization:	https://www.doi.org/10.1021/acs.jced.7b00920
Solid-Liquid Phase Equilibrium and Phase Diagram for the Ternary Carbamazepine-Succinic Acid-Ethanol or Acetone System at (298.15 and 308.15) K:	https://www.doi.org/10.1021/je100918d

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point