

Oxcarbazepine

Other names:	Trileptal 5H-Dibenz[b,f]azepine-5-carboxamide, 10,11-dihydro-10-oxo- 10,11-Dihydro-10-oxo-5H-dibenz[b,f]azepine-5-carboxamide GP-47680 10,11-Dihydro-10-oxo-5H-dibenz[b,f]azepin-5-carbonsaeureamid
Inchi:	InChI=1S/C15H12N2O2/c16-15(19)17-12-7-3-1-5-10(12)9-14(18)11-6-2-4-8-13(11)17/h1
InchiKey:	CTRLABGOLIVAIY-UHFFFAOYSA-N
Formula:	C15H12N2O2
SMILES:	NC(=O)N1c2ccccc2CC(=O)c2ccccc21
Mol. weight [g/mol]:	252.27
CAS:	28721-07-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.88		Crippen Method
logp	2.642		Crippen Method
mcvol	186.930	ml/mol	McGowan Method
rinpol	2490.40		NIST Webbook
rinpol	2490.40		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28721075&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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