

Carbamazepine, M(HO-ring), AC

Inchi: InChI=1S/C17H14N2O3/c1-11(20)22-14-8-9-16-13(10-14)7-6-12-4-2-3-5-15(12)19(16)17
InchiKey: HVAJMFMLCLSATN-UHFFFAOYSA-N
Formula: C17H14N2O3
SMILES: CC(=O)Oc1ccc2c(c1)C=Cc1ccccc1N2C(N)=O
Mol. weight [g/mol]: 294.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	3.313		Crippen Method
mcvol	216.680	ml/mol	McGowan Method
rinpole	2450.00		NIST Webbook
rinpole	2450.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R255533&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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