

5H-Dibenz[b,f]azepine-5-carboxamide, 10,11-dihydro-10-hydroxy-

Other names:

ALCOL RACEMO

10,11-Dihydro-10-hydroxycarbamazepine

Inchi:

InChI=1S/C15H14N2O2/c16-15(19)17-12-7-3-1-5-10(12)9-14(18)11-6-2-4-8-13(11)17/h1

InchiKey:

BMPDWHIDQYTSHX-UHFFFAOYSA-N

Formula:

C15H14N2O2

SMILES:

NC(=O)N1c2ccccc2CC(O)c2ccccc21

Mol. weight [g/mol]:

254.28

CAS:

29331-92-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	2.493		Crippen Method
mcvol	191.230	ml/mol	McGowan Method
rinpol	2527.90		NIST Webbook
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Sources

Crippen Method:

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

Crippen Method:

https://www.chemeo.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=C29331928&Units=SI>

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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