

Carbamazepine 10,11-epoxide

Other names:

6H-Dibenz[b,f]oxireno[d]azepine-6-carboxamide, 1a,10b-dihydro-
Carbamazepine 10,11-oxide
1a,10b-Dihydro-6H-dibenz(b,f)oxireno(d)azepine-6-carboxamide
10,11-Epoxy carbamazepine
GP 49-023
Carbamazepine epoxide

Inchi:

InChI=1S/C15H12N2O2/c16-15(18)17-11-7-3-1-5-9(11)13-14(19-13)10-6-2-4-8-12(10)17

InchiKey:

ZRWWEEVEIOGMMT-UHFFFAOYSA-N

Formula:

C15H12N2O2

SMILES:

NC(=O)N1c2ccccc2C2OC2c2ccccc21

Mol. weight [g/mol]:

252.27

CAS:

36507-30-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	3.029		Crippen Method
mcvol	180.370	ml/mol	McGowan Method

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C36507309&Units=SI>

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>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

mcvol:

McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/17-842-8/Carbamazepine-10-11-epoxide.pdf>

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