

5H-4,1-benzoxazepine-2,5-dione,1,2-dihydro-1-me

Other names:	5H-4,1-benzoxazepine-2,5-dione,1,2-dihydro-1-methyl
Inchi:	InChI=1S/C10H9NO3/c1-11-8-5-3-2-4-7(8)10(13)14-6-9(11)12/h2-5H,6H2,1H3
InchiKey:	DTWXADABYFWAHU-UHFFFAOYSA-N
Formula:	C10H9NO3
SMILES:	CN1C(=O)COC(=O)c2ccccc21
Mol. weight [g/mol]:	191.18
CAS:	3455-21-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.29		Crippen Method
logp	0.820		Crippen Method
mcvol	136.130	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3455218&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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