

2H-1,4Benzoxazin-6(8aH)-one, 3,4-dihydro-8a-hydroxy-4,7-dimethyl

Inchi:	InChI=1S/C10H13NO3/c1-7-6-10(13)9(5-8(7)12)11(2)3-4-14-10/h5-6,13H,3-4H2,1-2H3
InchiKey:	AMPLTVKIWKZEGO-UHFFFAOYSA-N
Formula:	C10H13NO3
SMILES:	CC1=CC2(O)OCCN(C)C2=CC1=O
Mol. weight [g/mol]:	195.22
CAS:	13033-37-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.81		Crippen Method
logp	0.050		Crippen Method
mcvol	144.730	ml/mol	McGowan Method

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=C13033379&Units=SI

Legend

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

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