

2H-1,2-Oxazine,tetrahydro-2-methyl-

Other names:	2-Methyl-[1,2]oxazinane
Inchi:	InChI=1S/C5H11NO/c1-6-4-2-3-5-7-6/h2-5H2,1H3
InchiKey:	PJMAADUWXUTYNS-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CN1CCCCO1
Mol. weight [g/mol]:	101.15
CAS:	22445-43-8

Physical Properties

Property code	Value	Unit	Source
ie	8.66	eV	NIST Webbook
log10ws	-0.46		Crippen Method
logp	0.644		Crippen Method
mcvol	86.300	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22445438&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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