

N-Propionylimidazole

Other names:	1H-Imidazole, 1-(1-oxopropyl)- 1-(1-oxopropyl)-1H-imidazole
Inchi:	InChI=1S/C6H8N2O/c1-2-6(9)8-4-3-7-5-8/h3-5H,2H2,1H3
InchiKey:	GDBUORNHWAZSNU-UHFFFAOYSA-N
Formula:	C6H8N2O
SMILES:	CCC(=O)n1ccnc1
Mol. weight [g/mol]:	124.14
CAS:	4122-52-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Crippen Method
logp	0.933		Crippen Method
mcvol	97.470	ml/mol	McGowan Method

Sources

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=C4122525&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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