

Pyrazineethanol

Inchi:	InChI=1S/C6H8N2O/c9-4-1-6-5-7-2-3-8-6/h2-3,5,9H,1,4H2
InchiKey:	MHDJZGMTVSLZDB-UHFFFAOYSA-N
Formula:	C6H8N2O
SMILES:	OCCc1cnccn1
Mol. weight [g/mol]:	124.14
CAS:	6705-31-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.07		Crippen Method
logp	0.011		Crippen Method
mcvol	97.470	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=C6705313&Units=SI

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/13-045-7/Pyrazineethanol.pdf>

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