

N-Methyl-L-prolinol

Other names:	(S)-(-)-1-Methyl-2-pyrrolidinemethanol (S)-(-)-2-Hydroxymethyl-1-methylpyrrolidine 2-Pyrrolidinemethanol, 1-methyl-, (S)- (S)-methylpyrrolidine-2-methanol
Inchi:	InChI=1S/C6H13NO/c1-7-4-2-3-6(7)5-8/h6,8H,2-5H2,1H3/t6-/m1/s1
InchiKey:	VCOJPHPOVDIRJK-ZCFIWIBFSA-N
Formula:	C6H13NO
SMILES:	CN1CCCC1CO
Mol. weight [g/mol]:	115.17
CAS:	34381-71-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.17		Crippen Method
logp	0.073		Crippen Method
mcvol	100.390	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.20	K	1.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34381710&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
tbrp:	Boiling point at reduced pressure

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