N-Methylloline

Inchi: InChI=1S/C9H16N2O/c1-10(2)8-7-5-11-4-3-6(12-7)9(8)11/h6-9H,3-5H2,1-2H3/t6-,7+,8-,9

InchiKey: FIWXXQWEVIQSAB-OBCZXFEGSA-N

Formula: C9H16N2O

SMILES: CN(C)C1C2CN3CCC(O2)C13

Mol. weight [g/mol]: 168.24

Physical Properties

Property code	Value	Unit	Source
log10ws	0.05		Crippen Method
logp	-0.228		Crippen Method
mcvol	130.920	ml/mol	McGowan Method
rinpol	1275.00		NIST Webbook
rinpol	1275.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R268336&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

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.