

1,1'-Methylenedipyrrolidine

Inchi: InChI=1S/C9H18N2/c1-2-6-10(5-1)9-11-7-3-4-8-11/h1-9H2
InchiKey: KQISQNCCCASDX-UHFFFAOYSA-N
Formula: C9H18N2
SMILES: C1CCN(CN2CCCC2)C1
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.01		Crippen Method
logp	1.136		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
rinsol	1054.00		NIST Webbook
rinsol	1054.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R573990&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

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<https://www.cheméo.com/cid/48-911-7/1-1-Methylenedipyrrolidine.pdf>

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