

Piperidine, 1-ethyl-3-methyl-

Other names: 1-ethyl-3-methylpiperidine
Inchi: InChI=1S/C8H17N/c1-3-9-6-4-5-8(2)7-9/h8H,3-7H2,1-2H3
InchiKey: YSPBEFPTFBRJBH-UHFFFAOYSA-N
Formula: C8H17N
SMILES: CCN1CCCC(C)C1
Mol. weight [g/mol]: 127.23
CAS: 2162-86-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.39		Crippen Method
logp	1.738		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
rinpol	908.00		NIST Webbook
ripol	1033.00		NIST Webbook
ripol	1033.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2162869&Units=SI>

Legend

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

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