Piperidine, 1-ethyl-2,6-dimethyl

Other names: 2,6-Dimethyl-1-ethyl piperidine
Inchi: InChI=1S/C9H19N/c1-4-10-8(2)6-5-7-9(10)3/h8-9H,4-7H2,1-3H3
InchiKey: HMVDCTBEKMKBIC-UHFFFAOYSA-N
Formula: C9H19N
SMILES: CCN1C(C)CCCC1C
Mol. weight [g/mol]: 141.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	2.269		Crippen Method
mcvol	136.790	ml/mol	McGowan Method
rinpol	993.00		NIST Webbook
rinpol	985.00		NIST Webbook
ripol	1126.00		NIST Webbook
ripol	1126.00		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=R222003&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