

Piperidine, 1-heptyl-3-methyl

Inchi: InChI=1S/C13H27N/c1-3-4-5-6-7-10-14-11-8-9-13(2)12-14/h13H,3-12H2,1-2H3
InchiKey: KTEVGDUPCGAFOZ-UHFFFAOYSA-N
Formula: C13H27N
SMILES: CCCCCCN1CCCC(C)C1
Mol. weight [g/mol]: 197.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	3.689		Crippen Method
mcvol	193.150	ml/mol	McGowan Method
rinpol	1371.00		NIST Webbook
ripol	1474.00		NIST Webbook

Sources

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=R222043&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

Latest version available from:

<https://www.chemeo.com/cid/61-436-0/Piperidine-1-heptyl-3-methyl.pdf>

Generated by Cheméo on 2024-05-01 03:15:10.99877479 +0000 UTC m=+16822559.919352105.

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