

N,3,5-Trimethylpiperidine

Inchi: InChI=1S/C8H17N/c1-7-4-8(2)6-9(3)5-7/h7-8H,4-6H2,1-3H3
InchiKey: IGJDIGJIINCEDE-UHFFFAOYSA-N
Formula: C8H17N
SMILES: CC1CC(C)CN(C)C1
Mol. weight [g/mol]: 127.23
CAS: 27644-32-2

Physical Properties

Property code	Value	Unit	Source
affp	978.10	kJ/mol	NIST Webbook
basg	947.20	kJ/mol	NIST Webbook
log10ws	-1.15		Crippen Method
logp	1.594		Crippen Method
mcvol	122.700	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C27644322&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/52-860-9/N-3-5-Trimethylpiperidine.pdf>

Generated by Cheméo on 2024-04-24 17:48:46.145134328 +0000 UTC m=+16270175.065711644.

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