

trans-1,3,5-Trimethylpiperidine

Inchi:	InChI=1S/C8H17N/c1-7-4-8(2)6-9(3)5-7/h7-8H,4-6H2,1-3H3/t7-,8-/m0/s1
InchiKey:	IGJDIGJIINCEDE-YUMQZZPRSA-N
Formula:	C8H17N
SMILES:	CC1CC(C)CN(C)C1
Mol. weight [g/mol]:	127.23
CAS:	16544-52-8

Physical Properties

Property code	Value	Unit	Source
ie	7.66 ± 0.05	eV	NIST Webbook
log10ws	-1.15		Crippen Method
logp	1.594		Crippen Method
mcvol	122.700	ml/mol	McGowan Method

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=C16544528&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/32-097-9/trans-1-3-5-Trimethylpiperidine.pdf>

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