

1-Isobutyl-piperidine

Other names:	Piperidine, 1-(2-methylpropyl)-
Inchi:	InChI=1S/C9H19N/c1-9(2)8-10-6-4-3-5-7-10/h9H,3-8H2,1-2H3
InchiKey:	BNBLWPUWMNURAX-UHFFFAOYSA-N
Formula:	C9H19N
SMILES:	CC(C)CN1CCCCC1
Mol. weight [g/mol]:	141.25
CAS:	10315-89-6

Physical Properties

Property code	Value	Unit	Source
affp	974.50	kJ/mol	NIST Webbook
basg	943.50	kJ/mol	NIST Webbook
ie	8.16 ± 0.03	eV	NIST Webbook
log10ws	-1.81		Crippen Method
logp	2.128		Crippen Method
mcvol	136.790	ml/mol	McGowan Method
rinpol	973.00		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=C10315896&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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