1-Isopentyl-piperidine

Other names:	N-Isopentylpiperidine
Inchi:	InChI=1S/C10H21N/c1-10(2)6-9-11-7-4-3-5-8-11/h10H,3-9H2,1-2H3
InchiKey:	PWMYYGYCTJRBBX-UHFFFAOYSA-N
Formula:	C10H21N
SMILES:	CC(C)CCN1CCCCC1
Mol. weight [g/mol]:	155.28
CAS:	4462-09-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.23		Crippen Method
logp	2.518		Crippen Method
mcvol	150.880	ml/mol	McGowan Method
rinpol	1080.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1084.00		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=C4462093&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

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