

N-(2-Methylpropyl)pyrrolidine

Other names:	1-(2'-Methylpropyl)pyrrolidine Pyrrolidine, 1-(2-methylpropyl)-
Inchi:	InChI=1S/C8H17N/c1-8(2)7-9-5-3-4-6-9/h8H,3-7H2,1-2H3
InchiKey:	KOFIDSXHWGFEMO-UHFFFAOYSA-N
Formula:	C8H17N
SMILES:	CC(C)CN1CCCC1
Mol. weight [g/mol]:	127.23
CAS:	39198-81-7

Physical Properties

Property code	Value	Unit	Source
ie	8.17 ± 0.03	eV	NIST Webbook
log10ws	-1.39		Crippen Method
logp	1.738		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
ripol	975.00		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C39198817&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

ripol: Polar retention indices

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