

Piperidine, 1-(1-oxo-2-butenyl)-

Other names:	Piperidine, 1-crotonoyl- N-Crotonylpiperidine 1-(1-oxobut-2-enyl)piperidine
Inchi:	InChI=1S/C9H15NO/c1-2-6-9(11)10-7-4-3-5-8-10/h2,6H,3-5,7-8H2,1H3
InchiKey:	DEHSTVNSEJEWPR-UHFFFAOYSA-N
Formula:	C9H15NO
SMILES:	CC=CC(=O)N1CCCCC1
Mol. weight [g/mol]:	153.22
CAS:	3626-69-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	1.575		Crippen Method
mcvol	134.060	ml/mol	McGowan Method

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=C3626695&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/20-018-9/Piperidine-1-1-oxo-2-butenyl.pdf>

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