

1-Azido-3-methylbutan-2-one

Inchi:	InChI=1S/C5H9N3O/c1-4(2)5(9)3-7-8-6/h4H,3H2,1-2H3
InchiKey:	IGJOEYTXYXBXLD-UHFFFAOYSA-N
Formula:	C5H9N3O
SMILES:	CC(C)C(=O)CN=[N+]=[N-]
Mol. weight [g/mol]:	127.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.04		Crippen Method
logp	1.522		Crippen Method
mcvol	104.220	ml/mol	McGowan Method

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=R412776&Units=SI

Legend

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

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