

3,3-Dimethyl-1-isopropyl diaziridine

Inchi: InChI=1S/C6H14N2/c1-5(2)8-6(3,4)7-8/h5,7H,1-4H3
InchiKey: XSBNZKOMEUOPFQ-UHFFFAOYSA-N
Formula: C6H14N2
SMILES: CC(C)N1NC1(C)C
Mol. weight [g/mol]: 114.19
CAS: 137675-05-9

Physical Properties

Property code	Value	Unit	Source
ie	8.98	eV	NIST Webbook
log10ws	-1.70		Crippen Method
logp	0.951		Crippen Method
mcvol	104.500	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=C137675059&Units=SI>

Legend

ie: Ionization energy
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/49-193-4/3-3-Dimethyl-1-isopropyl diaziridine.pdf>

Generated by Cheméo on 2024-05-03 00:45:14.182282732 +0000 UTC m=+16986363.102860048.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.