

Aziridinone, 1,3-bis(1,1-dimethylethyl)-

Other names:	2-Aziridinone, 1,3-di-tert-butyl- 1,3-Di-tert-butylaziridinone Aziridinone, 1,3-di-tert-butyl-
Inchi:	InChI=1S/C10H19NO/c1-9(2,3)7-8(12)11(7)10(4,5)6/h7H,1-6H3
InchiKey:	CEPIDWHUQBLHJH-UHFFFAOYSA-N
Formula:	C10H19NO
SMILES:	CC(C)(C)C1C(=O)N1C(C)(C)C
Mol. weight [g/mol]:	169.26
CAS:	14387-89-4

Physical Properties

Property code	Value	Unit	Source
ie	7.25	eV	NIST Webbook
ie	8.21	eV	NIST Webbook
log10ws	-2.23		Crippen Method
logp	2.042		Crippen Method
mcvol	152.450	ml/mol	McGowan Method

Sources

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=C14387894&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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