

Imidazoline, 1,3-dinitro-

Other names:	Imidazolidine, 1,3-dinitro- 1,3-Dinitro-2-methylimidazoline 1,3-Dinitroimidazolidine 1,3-Dinitro-tetrahydroimidazole 1,3-Dinitro-1,3-diazacyclopentane
Inchi:	InChI=1S/C3H6N4O4/c8-6(9)4-1-2-5(3-4)7(10)11/h1-3H2
InchiKey:	MGUHTGHCUOCIGG-UHFFFAOYSA-N
Formula:	C3H6N4O4
SMILES:	O=[N+]([O-])N1CCN([N+](=O)[O-])C1
Mol. weight [g/mol]:	162.10
CAS:	5754-91-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.76		Crippen Method
logp	-1.055		Crippen Method
mcvol	97.070	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=C5754916&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/81-304-4/Imidazoline-1-3-dinitro.pdf>

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