

2,4-Imidazolidinedione, 1-methyl-

Other names:	Hydantoin, 1-methyl- Dioxy-creatinine 1-Methylhydantoin 1-methyldiazolidine-2,4-dione
Inchi:	InChI=1S/C4H6N2O2/c1-6-2-3(7)5-4(6)8/h2H2,1H3,(H,5,7,8)
InchiKey:	RHYBFKMFHLPQPH-UHFFFAOYSA-N
Formula:	C4H6N2O2
SMILES:	CN1CC(=O)NC1=O
Mol. weight [g/mol]:	114.10
CAS:	616-04-6

Physical Properties

Property code	Value	Unit	Source
ie	9.30	eV	NIST Webbook
ie	9.57 ± 0.05	eV	NIST Webbook
log10ws	0.32		Crippen Method
logp	-0.832		Crippen Method
mvol	79.460	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=C616046&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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