

1-Bromo-3-chloro-5,5-dimethyl hydantoin

Other names:	1-bromo-3-chloro-5,5-dimethylimidazolidine-2,4-dione
Inchi:	InChI=1S/C5H6BrClN2O2/c1-5(2)3(10)8(7)4(11)9(5)6/h1-2H3
InchiKey:	PIEXCQIOSMOEOU-UHFFFAOYSA-N
Formula:	C5H6BrClN2O2
SMILES:	CC1(C)C(=O)N(Cl)C(=O)N1Br
Mol. weight [g/mol]:	241.47
CAS:	16079-88-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.16		Crippen Method
logp	1.493		Crippen Method
mcvol	123.290	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=C16079882&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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