

2,4-Imidazolidinedione, 1,3-bis(chloromethyl)-5,5-dimethyl-

Inchi:	InChI=1S/C7H10Cl2N2O2/c1-7(2)5(12)10(3-8)6(13)11(7)4-9/h3-4H2,1-2H3
InchiKey:	AQEGFWHPHETTH-UHFFFAOYSA-N
Formula:	C7H10Cl2N2O2
SMILES:	CC1(C)C(=O)N(CCI)C(=O)N1CCI
Mol. weight [g/mol]:	225.07
CAS:	116401-49-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.72		Crippen Method
logp	1.422		Crippen Method
mcvol	146.210	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=C116401491&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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