

1-Imidazolidinecarboxamide, n-(2-chloroethyl)-2-oxo-

Inchi:	InChI=1S/C6H10CIN3O2/c7-1-2-8-5(11)10-4-3-9-6(10)12/h1-4H2,(H,8,11)(H,9,12)
InchiKey:	HROMWFQVYBMXMS-UHFFFAOYSA-N
Formula:	C6H10CIN3O2
SMILES:	O=C(NCCCCI)N1CCNC1=O
Mol. weight [g/mol]:	191.62
CAS:	16813-33-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.84		Crippen Method
logp	-0.040		Crippen Method
mcvol	129.860	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16813335&Units=SI
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

Legend

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

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