

N-(Chloromethyl)phthalimide

Other names:	1H-Isoindole-1,3(2H)-dione, 2-(chloromethyl)-Chloromethylphthalimide N-Chloromethyltrimellitimide Phthalimide, N-(chloromethyl)- 4-Chloromethylphthalimide
Inchi:	InChI=1S/C9H6ClNO2/c10-5-11-8(12)6-3-1-2-4-7(6)9(11)13/h1-4H,5H2
InchiKey:	JKGLRGGCGUQNEX-UHFFFAOYSA-N
Formula:	C9H6ClNO2
SMILES:	O=C1c2ccccc2C(=O)N1CCl
Mol. weight [g/mol]:	195.60
CAS:	17564-64-6

Physical Properties

Property code	Value	Unit	Source
hsub	103.50 ± 1.10	kJ/mol	NIST Webbook
hsub	103.60 ± 0.90	kJ/mol	NIST Webbook
log10ws	-2.48		Crippen Method
logp	1.479		Crippen Method
mvol	128.410	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17564646&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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