

Phthalimide, n-chloro-

Other names:	N-chlorophthalimide
Inchi:	InChI=1S/C8H4ClNO2/c9-10-7(11)5-3-1-2-4-6(5)8(10)12/h1-4H
InchiKey:	WDRFYIPWHMGQPN-UHFFFAOYSA-N
Formula:	C8H4ClNO2
SMILES:	O=C1c2ccccc2C(=O)N1Cl
Mol. weight [g/mol]:	181.58
CAS:	3481-09-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	1.436		Crippen Method
mcvol	114.320	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=C3481092&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/32-018-6/Phthalimide-n-chloro.pdf>

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