N-(CHLOROMETHYL)PHTHALIMIDE

Other names:	1H-Isoindole-1,3(2H)-dione, 2-(chloromethyl)-
	4-Chloromethylphthalimide
	Chloromethylphthalimide
	N-Chloromethyltrimellitimide
	Phthalimide, N-(chloromethyl)-
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]:	195.61

Physical Properties

Property code	Value	Unit	Source
hf	-256.33	kJ/mol	Cheméo Relay (1.0)
hsub	103.50 ± 1.10	kJ/mol	NIST Webbook
hsub	103.60 ± 0.90	kJ/mol	NIST Webbook
ie	9.84	eV	Cheméo Relay (1.0)
logp	1.479		Crippen Method
mcvol	128.410	ml/mol	McGowan Method
tb	598.34	K	Cheméo Relay (1.0)
tf	406.60	K	Thermochemical study of some chloro and bromo alkyl substituted phthalimides: Structural energetic correlations

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17564646&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Thermochemical study of some chloro and bromo alkyl substituted phthalimides: Structural energetic correlations:	https://www.doi.org/10.1016/j.jct.2007.03.009

Legend

hf:	Enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point