4-CHLORO-1,8-NAPHTHALENEDICARBOXYLIC ANHYDRIDE

Other names: 4-Chloronaphthalic anhydride
1H,3H-Naphtho[1,8-cd]pyran-1,3-dione, 6-chloro-
4-chloronaphthalene-1,8-dicarboxylic anhydride

Inchi: InChI=1S/C12H5ClO3/c13-9-5-4-8-10-6(9)2-1-3-7(10)11(14)16-12(8)15/h1-5H

InchiKey: UJEUBSWHCGDJQU-UHFFFAOYSA-N

Formula: C12H5ClO3

SMILES: O=C1OC(=O)c2ccc(Cl)c3cccc1c23

Mol. weight [g/mol]: 232.62

Physical Properties

Property code	Value	Unit	Source
hf	-356.68	kJ/mol	Cheméo Relay (1.0)
hfus	24.99	kJ/mol	Joback Method
ie	8.98	eV	Cheméo Relay (1.0)
log10ws	-4.37		Cheméo Relay (1.0)
logp	2.804		Crippen Method
mcvol	147.110	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
tb	654.03	K	Cheméo Relay (1.0)
tc	967.61	K	Cheméo Relay (1.0)
tf	452.31	K	Cheméo Relay (1.0)
vc	0.552	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.11	J/mol×K	745.99	Joback Method
cpg	380.25	J/mol×K	791.74	Joback Method
cpg	390.41	J/mol×K	837.49	Joback Method
cpg	399.63	J/mol×K	883.24	Joback Method
cpg	407.93	J/mol×K	928.99	Joback Method
cpg	415.37	J/mol×K	974.74	Joback Method
cpg	421.98	J/mol×K	1020.48	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4053081&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume