Naphthalic anhydride

Other names:	1,8-Naphthalic anhydride
	1H,3H-Naphtho[1,8-cd]pyran-1,3-dione
	Naphthalic acid anhydride
	Protect
	1,8-Naphthalenedicarboxylic acid anhydride
	1,8-Naphthalenedicarboxylic anhydride
	1,8-Naphthalic acid anhydride
	Naphthalenedicarboxylic-1,8-anhydride
	Naphthalene-1,8-dicarboxylic acid anhydride
	1,8-Naphthoic anhydride
	Protect (agrochemical)
	Benzo[de]isochromene-1,3-dione
	1,8-Naphthanoic anhydride
	NSC 5747
	naphthalene-1,8-dicarboxylic anhydride
Inchi:	InChI=1S/C12H6O3/c13-11-8-5-1-3-7-4-2-6-9(10(7)8)12(14)15-11/h1-6H
InchiKey:	GRSMWKLPSNHDHA-UHFFFAOYSA-N
Formula:	C12H6O3
SMILES:	O=C1OC(=O)c2cccc3cccc1c23
Mol. weight [g/mol]:	198.17
CAS:	81-84-5

Physical Properties

Property code	Value	Unit	Source
gf	-12.88	kJ/mol	Joback Method
hf	-200.61	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Joback Method
hvap	60.77	kJ/mol	Joback Method
ie	8.92 ± 0.05	eV	NIST Webbook
log10ws	-3.73		Crippen Method
logp	2.150		Crippen Method
mcvol	134.870	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
rinpol	340.80		NIST Webbook
rinpol	339.90		NIST Webbook
rinpol	342.17		NIST Webbook
rinpol	1944.00		NIST Webbook

rinpol	342.17		NIST Webbook
rinpol	1944.00		NIST Webbook
rinpol	339.20		NIST Webbook
rinpol	341.19		NIST Webbook
tb	703.58	K	Joback Method
tc	975.82	K	Joback Method
tf	545.70 ± 0.20	K	NIST Webbook
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.21	J/mol×K	703.58	Joback Method
cpg	362.66	J/mol×K	748.95	Joback Method
cpg	374.06	J/mol×K	794.33	Joback Method
cpg	384.47	J/mol×K	839.70	Joback Method
cpg	393.92	J/mol×K	885.07	Joback Method
cpg	402.46	J/mol×K	930.44	Joback Method
cpg	410.14	J/mol×K	975.82	Joback Method
hfust	23.32	kJ/mol	542.30	NIST Webbook
hfust	23.32	kJ/mol	542.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C81845&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume