1H-Benz[de]isoquinoline-1,3(2H)-dione

Other names:	Naphthalimide
	1,8-Naphthalenedicarboximide
	1,8-Naphthalimide
	naphthalene-1,8-dicarboximide
Inchi:	InChI=1S/C12H7NO2/c14-11-8-5-1-3-7-4-2-6-9(10(7)8)12(15)13-11/h1-6H,(H,13,14,15)
InchiKey:	XJHABGPPCLHLLV-UHFFFAOYSA-N
Formula:	C12H7NO2
SMILES:	O=C1N=C(O)c2cccc3cccc1c23
Mol. weight [g/mol]:	197.19
CAS:	81-83-4

Physical Properties

Property code	Value	Unit	Source
gf	196.12	kJ/mol	Joback Method
hf	34.14	kJ/mol	Joback Method
hfus	23.75	kJ/mol	Joback Method
hvap	75.86	kJ/mol	Joback Method
ie	8.68 ± 0.05	eV	NIST Webbook
log10ws	-3.38		Crippen Method
logp	2.298		Crippen Method
mcvol	138.980	ml/mol	McGowan Method
pc	4374.18	kPa	Joback Method
tb	758.83	K	Joback Method
tc	1006.53	K	Joback Method
tf	545.20	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.32	J/mol×K	758.83	Joback Method
cpg	394.80	J/mol×K	800.11	Joback Method
cpg	404.40	J/mol×K	841.40	Joback Method
cpg	413.19	J/mol×K	882.68	Joback Method

cpg	421.22	J/mol×K	923.96	Joback Method
cpg	428.55	J/mol×K	965.25	Joback Method
cpg	435.23	J/mol×K	1006.53	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81834&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume