3,6-Diaminophthalimide

Inchi: InChI=1S/C8H7N3O2/c9-3-1-2-4(10)6-5(3)7(12)11-8(6)13/h1-2H,9-10H2,(H,11,12,13)
InchiKey: GNDGADUBGMTBEC-UHFFFAOYSA-N
Formula: C8H7N3O2
SMILES: Nc1ccc(N)c2c1C(=O)NC2=O
Mol. weight [g/mol]: 177.16
CAS: 1660-15-7

Physical Properties

Property code	Value	Unit	Source
gf	143.89	kJ/mol	Joback Method
hf	-83.20	kJ/mol	Joback Method
hfus	25.42	kJ/mol	Joback Method
hvap	74.42	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	-0.265		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
pc	5670.27	kPa	Joback Method
tb	764.72	K	Joback Method
tc	1044.11	K	Joback Method
tf	674.07	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.44	J/mol×K	764.72	Joback Method
cpg	346.22	J/mol×K	811.28	Joback Method
cpg	355.97	J/mol×K	857.85	Joback Method
cpg	364.65	J/mol×K	904.41	Joback Method
cpg	372.21	J/mol×K	950.98	Joback Method
cpg	378.61	J/mol×K	997.54	Joback Method
cpg	383.80	J/mol×K	1044.11	Joback Method
hsubt	98.50	kJ/mol	484.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1660157&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
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