phthalamide

Inchi: InChI=1S/C8H7NO2/c10-7-5-3-1-2-4-6(5)8(11)9-7/h1-6H,(H,9,10,11)
InchiKey: RDHHZPRHIKNBBI-UHFFFAOYSA-N
Formula: C8H7NO2
SMILES: O=C1NC(=O)C2C=CC=CC12
Mol. weight [g/mol]: 149.15

Physical Properties

Property code	Value	Unit	Source
gf	4.13	kJ/mol	Joback Method
hf	-203.36	kJ/mol	Joback Method
hfus	17.50	kJ/mol	Joback Method
hvap	49.58	kJ/mol	Joback Method
log10ws	-2.93		Aqueous Solubility Prediction Method
log10ws	-2.93		Estimated Solubility Method
logp	0.001		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
tb	591.24	K	Joback Method
tc	856.34	K	Joback Method
tf	448.23	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.61	J/mol×K	591.24	Joback Method
cpg	279.63	J/mol×K	635.42	Joback Method
cpg	293.67	J/mol×K	679.61	Joback Method
cpg	306.72	J/mol×K	723.79	Joback Method
cpg	318.73	J/mol×K	767.97	Joback Method
cpg	329.69	J/mol×K	812.16	Joback Method
cpg	339.55	J/mol×K	856.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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
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