1H-Isoindole-1,3(2H)-dione, 5-amino-

Other names: 4-Aminophthalimide
Phthalimide, 4-amino-
Isoindole, 1,3(2H)-dione, 5-amino-
Inchi: InChI=1S/C8H6N2O2/c9-4-1-2-5-6(3-4)8(12)10-7(5)11/h1-3H,9H2,(H,10,11,12)
InchiKey: PXRKCOCTEMYUEG-UHFFFAOYSA-N
Formula: C8H6N2O2
SMILES: Nc1ccc2c(c1)C(=O)NC2=O
Mol. weight [g/mol]: 162.15
CAS: 3676-85-5

Physical Properties

Property code	Value	Unit	Source
gf	87.07	kJ/mol	Joback Method
hf	-105.52	kJ/mol	Joback Method
hfus	20.61	kJ/mol	Joback Method
hvap	63.12	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	0.152		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	5327.93	kPa	Joback Method
tb	687.21	K	Joback Method
tc	962.71	K	Joback Method
tf	578.29	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.25	J/mol×K	687.21	Joback Method
cpg	297.78	J/mol×K	733.13	Joback Method
cpg	308.42	J/mol×K	779.04	Joback Method
cpg	318.13	J/mol×K	824.96	Joback Method
cpg	326.88	J/mol×K	870.88	Joback Method
cpg	334.62	J/mol×K	916.79	Joback Method

cpg	341.32	J/mol×K	962.71	Joback Method
hsubt	135.30	kJ/mol	471.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3676855&Units=SI

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