3-Acetamidophthalimide

Inchi: InChI=1S/C10H8N2O3/c1-5(13)11-7-4-2-3-6-8(7)10(15)12-9(6)14/h2-4H,1H3,(H,11,13)(H
InchiKey: SJRJIOQDTLOAQV-UHFFFAOYSA-N
Formula: C10H8N2O3
SMILES: CC(=O)Nc1cccc2c1C(=O)NC2=O
Mol. weight [g/mol]: 204.18
CAS: 6118-65-6

Physical Properties

Property code	Value	Unit	Source
gf	-2.07	kJ/mol	Joback Method
hf	-239.70	kJ/mol	Joback Method
hfus	27.29	kJ/mol	Joback Method
hvap	70.11	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	0.529		Crippen Method
mcvol	141.810	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
tb	764.48	K	Joback Method
tc	1022.96	K	Joback Method
tf	620.16	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.46	J/mol×K	764.48	Joback Method
cpg	400.15	J/mol×K	807.56	Joback Method
cpg	410.79	J/mol×K	850.64	Joback Method
cpg	420.34	J/mol×K	893.72	Joback Method
cpg	428.77	J/mol×K	936.80	Joback Method
cpg	436.08	J/mol×K	979.88	Joback Method
cpg	442.23	J/mol×K	1022.96	Joback Method
hsubt	108.50	kJ/mol	448.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6118656&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