2-Amino-3,4,6-trichlorophenol

Inchi: InChI=1S/C6H4Cl3NO/c7-2-1-3(8)6(11)5(10)4(2)9/h1,11H,10H2
InchiKey: QQDKXJSYZGJGKJ-UHFFFAOYSA-N
Formula: C6H4Cl3NO
SMILES: Nc1c(O)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 212.46
CAS: 6358-15-2

Physical Properties

Property code	Value	Unit	Source
gf	-40.80	kJ/mol	Joback Method
hf	-155.79	kJ/mol	Joback Method
hfus	27.74	kJ/mol	Joback Method
hvap	70.02	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.935		Crippen Method
mcvol	124.210	ml/mol	McGowan Method
pc	5008.59	kPa	Joback Method
tb	643.74	K	Joback Method
tc	903.52	K	Joback Method
tf	506.10	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.86	J/mol×K	643.74	Joback Method
cpg	248.85	J/mol×K	687.04	Joback Method
cpg	254.40	J/mol×K	730.33	Joback Method
cpg	259.59	J/mol×K	773.63	Joback Method
cpg	264.52	J/mol×K	816.93	Joback Method
cpg	269.26	J/mol×K	860.23	Joback Method
cpg	273.92	J/mol×K	903.52	Joback Method

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=C6358152&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
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