Benzoic acid, 3-amino-2,5-dichloro-

Inchi: InChI=1S/C7H5Cl2NO2/c8-3-1-2-4(10)6(9)5(3)7(11)12/h1-2H,10H2,(H,11,12)
InchiKey: SVMCPPLCIXHWBS-UHFFFAOYSA-N
Formula: C7H5Cl2NO2
SMILES: Nc1ccc(Cl)c(C(=O)O)c1Cl
Mol. weight [g/mol]: 206.03
CAS: 50917-29-8

Physical Properties

Property code	Value	Unit	Source
gf	-131.57	kJ/mol	Joback Method
hf	-248.19	kJ/mol	Joback Method
hfus	26.04	kJ/mol	Joback Method
hvap	78.27	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.274		Crippen Method
mcvol	127.630	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
tb	694.62	K	Joback Method
tc	921.79	K	Joback Method
tf	486.48	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.93	J/mol×K	694.62	Joback Method
cpg	280.35	J/mol×K	732.48	Joback Method
cpg	286.29	J/mol×K	770.34	Joback Method
cpg	291.76	J/mol×K	808.21	Joback Method
cpg	296.79	J/mol×K	846.07	Joback Method
cpg	301.40	J/mol×K	883.93	Joback Method
cpg	305.59	J/mol×K	921.79	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=C50917298&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