3,5-Dichloro-4-aminobenzoic acid

Other names: 3,5-dichloro-4-oxo-4H-pyridine-1-acetic acid
Inchi: InChI=1S/C7H5Cl2NO2/c8-4-1-3(7(11)12)2-5(9)6(4)10/h1-2H,10H2,(H,11,12)
InchiKey: UHXYYTSWBYTDPD-UHFFFAOYSA-N
Formula: C7H5Cl2NO2
SMILES: Nc1c(Cl)cc(C(=O)O)cc1Cl
Mol. weight [g/mol]: 206.03

Physical Properties

Property code	Value	Unit	Source
hf	-350.94	kJ/mol	Cheméo Relay (1.0)
hfus	26.04	kJ/mol	Joback Method
ie	8.46	eV	Cheméo Relay (1.0)
log10ws	-3.03		Cheméo Relay (1.0)
logp	2.274		Crippen Method
mcvol	127.630	ml/mol	McGowan Method
tb	575.49	K	Cheméo Relay (1.0)
tf	517.74	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56187372&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point