Benzonitrile, 4-amino-3,5-dichloro-

Other names: 4-amino-3,5-dichlorobenzonitrile
Inchi: InChI=1S/C7H4Cl2N2/c8-5-1-4(3-10)2-6(9)7(5)11/h1-2H,11H2
InchiKey: COFNCCWGWXFACE-UHFFFAOYSA-N
Formula: C7H4Cl2N2
SMILES: N#Cc1cc(Cl)c(N)c(Cl)c1
Mol. weight [g/mol]: 187.03
CAS: 78473-00-4

Physical Properties

Property code	Value	Unit	Source
gf	267.35	kJ/mol	Joback Method
hf	181.50	kJ/mol	Joback Method
hfus	21.86	kJ/mol	Joback Method
hvap	65.33	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.447		Crippen Method
mcvol	121.570	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
tb	650.65	K	Joback Method
tc	905.93	K	Joback Method
tf	440.72	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.01	J/mol×K	650.65	Joback Method
cpg	246.84	J/mol×K	693.20	Joback Method
cpg	253.15	J/mol×K	735.74	Joback Method
cpg	258.95	J/mol×K	778.29	Joback Method
cpg	264.26	J/mol×K	820.84	Joback Method
cpg	269.11	J/mol×K	863.39	Joback Method
cpg	273.52	J/mol×K	905.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78473004&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

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