4-Amino-3-chloro-5-methyl benzonitrile

Inchi: InChI=1S/C8H7ClN2/c1-5-2-6(4-10)3-7(9)8(5)11/h2-3H,11H2,1H3
InchiKey: NDTNVCCDQAOBSZ-UHFFFAOYSA-N
Formula: C8H7ClN2
SMILES: Cc1cc(C#N)cc(Cl)c1N
Mol. weight [g/mol]: 166.61
CAS: 158296-69-6

Physical Properties

Property code	Value	Unit	Source
gf	287.70	kJ/mol	Joback Method
hf	176.60	kJ/mol	Joback Method
hfus	20.25	kJ/mol	Joback Method
hvap	63.17	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.102		Crippen Method
mcvol	123.420	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
tb	636.10	K	Joback Method
tc	882.91	K	Joback Method
tf	422.07	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.85	J/mol×K	636.10	Joback Method
cpg	275.59	J/mol×K	677.24	Joback Method
cpg	283.74	J/mol×K	718.37	Joback Method
cpg	291.31	J/mol×K	759.51	Joback Method
cpg	298.32	J/mol×K	800.64	Joback Method
cpg	304.81	J/mol×K	841.78	Joback Method
cpg	310.77	J/mol×K	882.91	Joback Method

Sources

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=C158296696&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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