4-Amino-3-chlorobenzonitrile

Inchi: InChI=1S/C7H5ClN2/c8-6-3-5(4-9)1-2-7(6)10/h1-3H,10H2
InchiKey: OREVCMGFYSUYPX-UHFFFAOYSA-N
Formula: C7H5ClN2
SMILES: N#Cc1ccc(N)c(Cl)c1
Mol. weight [g/mol]: 152.58
CAS: 21803-75-8

Physical Properties

Property code	Value	Unit	Source
gf	288.91	kJ/mol	Joback Method
hf	208.71	kJ/mol	Joback Method
hfus	18.05	kJ/mol	Joback Method
hvap	60.28	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.794		Crippen Method
mcvol	109.330	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	608.24	K	Joback Method
tc	859.69	K	Joback Method
tf	398.28	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.84	J/mol×K	608.24	Joback Method
cpg	231.65	J/mol×K	650.15	Joback Method
cpg	238.88	J/mol×K	692.06	Joback Method
cpg	245.54	J/mol×K	733.97	Joback Method
cpg	251.68	J/mol×K	775.87	Joback Method
cpg	257.31	J/mol×K	817.78	Joback Method
cpg	262.46	J/mol×K	859.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21803758&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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