3-Chloro-2-methylbenzonitrile

Inchi: InChI=1S/C8H6ClN/c1-6-7(5-10)3-2-4-8(6)9/h2-4H,1H3
InchiKey: FKFZTNLSUJCIMG-UHFFFAOYSA-N
Formula: C8H6ClN
SMILES: Cc1c(Cl)cccc1C#N
Mol. weight [g/mol]: 151.59
CAS: 54454-12-5

Physical Properties

Property code	Value	Unit	Source
gf	230.88	kJ/mol	Joback Method
hf	154.28	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	51.86	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.520		Crippen Method
mcvol	113.440	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
tb	558.59	K	Joback Method
tc	797.23	K	Joback Method
tf	326.29	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.61	J/mol×K	558.59	Joback Method
cpg	230.58	J/mol×K	598.36	Joback Method
cpg	238.96	J/mol×K	638.14	Joback Method
cpg	246.78	J/mol×K	677.91	Joback Method
cpg	254.06	J/mol×K	717.68	Joback Method
cpg	260.81	J/mol×K	757.46	Joback Method
cpg	267.08	J/mol×K	797.23	Joback Method

Sources

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=C54454125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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