3,5-Dichloro-4-hydroxybenzonitrile

Other names: Benzonitrile, 3,5-dichloro-4-hydroxy-
Inchi: InChI=1S/C7H3Cl2NO/c8-5-1-4(3-10)2-6(9)7(5)11/h1-2,11H
InchiKey: YRSSHOVRSMQULE-UHFFFAOYSA-N
Formula: C7H3Cl2NO
SMILES: N#Cc1cc(Cl)c(O)c(Cl)c1
Mol. weight [g/mol]: 188.01
CAS: 1891-95-8

Physical Properties

Property code	Value	Unit	Source
gf	55.91	kJ/mol	Joback Method
hf	-18.13	kJ/mol	Joback Method
hfus	22.83	kJ/mol	Joback Method
hvap	67.04	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.571		Crippen Method
mcvol	117.460	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
tb	653.76	K	Joback Method
tc	910.50	K	Joback Method
tf	456.66	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.72	J/mol×K	653.76	Joback Method
cpg	237.49	J/mol×K	696.55	Joback Method
cpg	242.83	J/mol×K	739.34	Joback Method
cpg	247.82	J/mol×K	782.13	Joback Method
cpg	252.57	J/mol×K	824.92	Joback Method
cpg	257.16	J/mol×K	867.71	Joback Method
cpg	261.68	J/mol×K	910.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1891958&Units=SI

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