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

Physical Properties

Property code	Value	Unit	Source
hfus	22.83	kJ/mol	Joback Method
hvap	75.78	kJ/mol	Cheméo Relay (1.0)
ie	9.34	eV	Cheméo Relay (1.0)
log10ws	-2.64		Cheméo Relay (1.0)
logp	2.571		Crippen Method
mcvol	117.460	ml/mol	McGowan Method
tb	506.08	K	Cheméo Relay (1.0)
tf	409.44	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1891958&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point