3,5-DICHLOROBENZONITRILE

Other names: Benzonitrile, 3,5-dichloro-
Inchi: InChI=1S/C7H3Cl2N/c8-6-1-5(4-10)2-7(9)3-6/h1-3H
InchiKey: PUJSUOGJGIECFQ-UHFFFAOYSA-N
Formula: C7H3Cl2N
SMILES: N#Cc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 172.01

Physical Properties

Property code	Value	Unit	Source
ea	0.80 ± 0.09	eV	NIST Webbook
ea	0.83 ± 0.09	eV	NIST Webbook
hf	153.57	kJ/mol	Cheméo Relay (1.0)
hfus	17.05	kJ/mol	Joback Method
hvap	65.28	kJ/mol	Cheméo Relay (1.0)
ie	9.95	eV	Cheméo Relay (1.0)
log10ws	-3.34		Cheméo Relay (1.0)
logp	2.865		Crippen Method
mcvol	111.590	ml/mol	McGowan Method
tb	513.67	K	Cheméo Relay (1.0)
tf	354.85	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.82	J/mol×K	573.14	Joback Method
cpg	205.80	J/mol×K	614.43	Joback Method
cpg	212.24	J/mol×K	655.72	Joback Method
cpg	218.19	J/mol×K	697.01	Joback Method
cpg	223.66	J/mol×K	738.31	Joback Method
cpg	228.67	J/mol×K	779.60	Joback Method
cpg	233.27	J/mol×K	820.89	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6575004&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

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
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