Benzonitrile, 2,6-dichloro-

Other names:	2,6-DBN
	2,6-Dichlorbenzonitril
	2,6-Dichlorobenzoic acid nitrile
	2,6-Dichlorobenzonitrile
	BH Prefix D
	Carsoron
	Casaron
	Casoron
	Casoron 133
	Casoron G
	Casoron G4
	Code H 133
	DBN
	DBN (pesticide)
	DBN (the herbicide)
	Decabane
	Dichlobenil
	Du-Sprex
	H 1313
	H 133
	NSC 521490
	Nia 5996
	Niagara 5,996
	Niagara 5006
	Prefix D
	Surfassol
Inchi:	InChI=1S/C7H3Cl2N/c8-6-2-1-3-7(9)5(6)4-10/h1-3H
InchiKey:	YOYAIZYFCNQIRF-UHFFFAOYSA-N
Formula:	C7H3Cl2N
SMILES:	N#Cc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	172.01
CAS:	1194-65-6

Physical Properties

Property code	Value	Unit	Source
ea	0.70 ± 0.09	eV	NIST Webbook

gf	210.53	kJ/mol	Joback Method
hf	159.18	kJ/mol	Joback Method
hfus	17.05	kJ/mol	Joback Method
hvap	54.02	kJ/mol	Joback Method
ie	10.09 ± 0.05	eV	NIST Webbook
log10ws	-4.24		Aqueous Solubility Prediction Method
logp	2.865		Crippen Method
mcvol	111.590	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
rinpol	1284.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1345.00		NIST Webbook
ripol	2084.00		NIST Webbook
ripol	2084.00		NIST Webbook
ripol	2084.00		NIST Webbook
tb	573.14	K	Joback Method
tc	820.89	K	Joback Method
tf	417.24 ± 0.20	K	NIST Webbook
tf	417.27	K	Aqueous Solubility Prediction Method
tf	416.70 ± 0.20	K	NIST Webbook
vc	0.444	m3/kmol	Joback Method

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
hfust	24.56	kJ/mol	421.20	NIST Webbook
hfust	26.17	kJ/mol	417.20	NIST Webbook
hfust	26.17	kJ/mol	417.20	NIST Webbook

hfust	25.94	kJ/mol	416.70	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1194656&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume