Chloroneb

Other names:	1,4-Dichloro-2,5-dimethoxybenzene
	Benzene, 1,4-dichloro-2,5-dimethoxy-
	Chloronebe
	Demasan
	Demosan
	Demosan 65W
	NSC 151546
	Soil Fungicide 1823
	Terraneb SP
	Tersan SP
Inchi:	InChI=1S/C8H8Cl2O2/c1-11-7-3-6(10)8(12-2)4-5(7)9/h3-4H,1-2H3
InchiKey:	PFIADAMVCJPXSF-UHFFFAOYSA-N
Formula:	C8H8Cl2O2
SMILES:	COc1cc(Cl)c(OC)cc1Cl
Mol. weight [g/mol]:	207.05
CAS:	2675-77-6

Physical Properties

Property code	Value	Unit	Source
gf	-133.86	kJ/mol	Joback Method
hf	-302.25	kJ/mol	Joback Method
hfus	20.12	kJ/mol	Joback Method
hvap	51.25	kJ/mol	Joback Method
log10ws	-4.41		Aqueous Solubility Prediction Method
logp	3.011		Crippen Method
mcvol	136.040	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	1508.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1508.00		NIST Webbook
tb	543.76	K	Joback Method
tc	765.36	K	Joback Method
tf	404.40 ± 0.20	K	NIST Webbook

tf	404.16 ± 0.20	K	NIST Webbook
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.19	J/mol×K	728.42	Joback Method
cpg	321.89	J/mol×K	765.36	Joback Method
cpg	268.48	J/mol×K	543.76	Joback Method
cpg	278.53	J/mol×K	580.69	Joback Method
cpg	288.14	J/mol×K	617.63	Joback Method
cpg	297.29	J/mol×K	654.56	Joback Method
cpg	305.98	J/mol×K	691.49	Joback Method
dvisc	0.0001753	Pa×s	543.76	Joback Method
dvisc	0.0002098	Pa×s	511.17	Joback Method
dvisc	0.0008515	Pa×s	348.20	Joback Method
dvisc	0.0005846	Pa×s	380.79	Joback Method
dvisc	0.0004258	Pa×s	413.39	Joback Method
dvisc	0.0003249	Pa×s	445.98	Joback Method
dvisc	0.0002572	Pa×s	478.57	Joback Method
hfust	27.56	kJ/mol	403.90	NIST Webbook
hfust	27.56	kJ/mol	403.90	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2675776&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume