Dibenzo[b,e][1,4]dioxin, 1-chloro-

Other names:	1-Chlorodibenzo-p-dioxin
	Dibenzo-p-dioxin, 1-chloro-
	1-Chlorodibenzodioxin
	1-Chlorodibenzo[b,e] [1,4]dioxin
Inchi:	InChI=1S/C12H7ClO2/c13-8-4-3-7-11-12(8)15-10-6-2-1-5-9(10)14-11/h1-7H
InchiKey:	VGGGRWRBGXENKI-UHFFFAOYSA-N
Formula:	C12H7ClO2
SMILES:	Clc1cccc2c1Oc1ccccc1O2
Mol. weight [g/mol]:	218.64
CAS:	39227-53-7

Physical Properties

Property code	Value	Unit	Source
gf	142.48	kJ/mol	Joback Method
hf	-32.80	kJ/mol	Joback Method
hfus	33.07	kJ/mol	Joback Method
hsub	95.20 ± 1.10	kJ/mol	NIST Webbook
hvap	62.30	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	4.238		Crippen Method
mcvol	145.540	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
rinpol	1811.00		NIST Webbook
rinpol	1812.00		NIST Webbook
tb	640.73	K	Joback Method
tc	899.71	K	Joback Method
tf	378.00 ± 1.00	K	NIST Webbook
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.98	J/mol×K	856.54	Joback Method
cpg	394.59	J/mol×K	899.71	Joback Method

cpg	338.40	J/mol×K	640.73	Joback Method
cpg	349.94	J/mol×K	683.89	Joback Method
cpg	360.45	J/mol×K	727.06	Joback Method
cpg	370.04	J/mol×K	770.22	Joback Method
cpg	378.84	J/mol×K	813.38	Joback Method
dvisc	0.0006035	Pa×s	604.63	Joback Method
dvisc	0.0005249	Pa×s	640.73	Joback Method
dvisc	0.0017305	Pa×s	424.16	Joback Method
dvisc	0.0013121	Pa×s	460.25	Joback Method
dvisc	0.0010357	Pa×s	496.35	Joback Method
dvisc	0.0008442	Pa×s	532.45	Joback Method
dvisc	0.0007062	Pa×s	568.54	Joback Method
hfust	23.20	kJ/mol	378.20	NIST Webbook
hsubt	98.60	kJ/mol	320.50	NIST Webbook
hsubt	100.50 ± 0.80	kJ/mol	325.50	NIST Webbook

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=C39227537&Units=SI

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
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation 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