Dibenzo[b,e][1,4]dioxin, 1,2,4-trichloro-

Other names:	1,2,4-Trichlorodibenzo-p-dioxin
	1,2,4-Trichlorodibenzo-para-dioxin
	1,2,4-Trichlorodibenzo[b,e] [1,4]dioxin
	1,2,4-Trichlorodibenzodioxin
	1,2,4-trichlorooxanthrene
	Dibenzo-p-dioxin, 1,2,4-trichloro-
Inchi:	InChI=1S/C12H5Cl3O2/c13-6-5-7(14)11-12(10(6)15)17-9-4-2-1-3-8(9)16-11/h1-5H
InchiKey:	HRVUKLBFRPWXPJ-UHFFFAOYSA-N
Formula:	C12H5Cl3O2
SMILES:	Clc1cc(Cl)c2c(c1Cl)Oc1ccccc1O2
Mol. weight [g/mol]:	287.53
CAS:	39227-58-2

Physical Properties

Property code	Value	Unit	Source
gf	99.36	kJ/mol	Joback Method
hf	-87.22	kJ/mol	Joback Method
hfus	40.69	kJ/mol	Joback Method
hvap	72.39	kJ/mol	Joback Method
log10ws	-7.60		Aqueous Solubility Prediction Method
logp	5.545		Crippen Method
mcvol	170.020	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	2152.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2143.00		NIST Webbook
rinpol	2143.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	725.55	K	Joback Method
tc	990.47	K	Joback Method
tf	509.04	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.56	J/mol×K	946.32	Joback Method
cpg	419.96	J/mol×K	990.47	Joback Method
cpg	374.96	J/mol×K	725.55	Joback Method
cpg	383.94	J/mol×K	769.70	Joback Method
cpg	392.18	J/mol×K	813.86	Joback Method
cpg	399.78	J/mol×K	858.01	Joback Method
cpg	406.87	J/mol×K	902.16	Joback Method
dvisc	0.0004903	Pa×s	725.55	Joback Method
dvisc	0.0005557	Pa×s	689.47	Joback Method
dvisc	0.0013574	Pa×s	509.04	Joback Method
dvisc	0.0010829	Pa×s	545.13	Joback Method
dvisc	0.0008885	Pa×s	581.21	Joback Method
dvisc	0.0007461	Pa×s	617.30	Joback Method
dvisc	0.0006387	Pa×s	653.38	Joback Method
hsubt	118.80	kJ/mol	342.00	NIST Webbook
hsubt	121.00 ± 1.80	kJ/mol	365.50	NIST Webbook

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C39227582&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

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

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