

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:	HRVUKLBFRPWPXJ-UHFFFAOYSA-N
Formula:	C12H5Cl3O2
SMILES:	Clc1cc(Cl)c2c(c1Cl)Oc1cccc1O2
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	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2143.00		NIST Webbook
rinpol	2143.00		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	374.96	J/molxK	725.55	Joback Method
cpg	383.94	J/molxK	769.70	Joback Method
cpg	392.18	J/molxK	813.86	Joback Method
cpg	399.78	J/molxK	858.01	Joback Method
cpg	406.87	J/molxK	902.16	Joback Method
cpg	413.56	J/molxK	946.32	Joback Method
cpg	419.96	J/molxK	990.47	Joback Method
dvisc	0.0010829	Paxs	545.13	Joback Method
dvisc	0.0013574	Paxs	509.04	Joback Method
dvisc	0.0008885	Paxs	581.21	Joback Method
dvisc	0.0007461	Paxs	617.30	Joback Method
dvisc	0.0006387	Paxs	653.38	Joback Method
dvisc	0.0005557	Paxs	689.47	Joback Method
dvisc	0.0004903	Paxs	725.55	Joback Method
hsubt	121.00 ± 1.80	kJ/mol	365.50	NIST Webbook
hsubt	118.80	kJ/mol	342.00	NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C39227582&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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
rinqol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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