

Dibenzo[b,e][1,4]dioxin, 2,3-dichloro-

Other names:	Dibenzo-p-dioxin, 2,3-dichloro- 2,3-Dichlorodibenzo-p-dioxin 2,3-Dichlorodibenzodioxin 2,3-Dichlorodibenzo-para-dioxin 2,3-Dichlorodibenzo[b,e] [1,4]dioxin
Inchi:	InChI=1S/C12H6Cl2O2/c13-7-5-11-12(6-8(7)14)16-10-4-2-1-3-9(10)15-11/h1-6H
InchiKey:	YCIYTXRUZSDMRZ-UHFFFAOYSA-N
Formula:	C12H6Cl2O2
SMILES:	Clc1cc2c(cc1Cl)Oc1ccccc1O2
Mol. weight [g/mol]:	253.08
CAS:	29446-15-9

Physical Properties

Property code	Value	Unit	Source
gf	120.92	kJ/mol	Joback Method
hf	-60.01	kJ/mol	Joback Method
hfus	36.88	kJ/mol	Joback Method
hsub	108.60 ± 1.00	kJ/mol	NIST Webbook
hsub	108.60 ± 1.00	kJ/mol	NIST Webbook
hvap	67.35	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.891		Crippen Method
mcvol	157.780	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	328.39		NIST Webbook
rinpol	328.39		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	2016.00		NIST Webbook
rinpol	2015.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	1984.00		NIST Webbook
tb	683.14	K	Joback Method
tc	945.37	K	Joback Method
tf	466.60	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.86	J/mol×K	901.66	Joback Method
cpg	377.11	J/mol×K	770.55	Joback Method
cpg	367.82	J/mol×K	726.84	Joback Method
cpg	357.63	J/mol×K	683.14	Joback Method
cpg	385.63	J/mol×K	814.25	Joback Method
cpg	407.80	J/mol×K	945.37	Joback Method
cpg	393.51	J/mol×K	857.96	Joback Method
dvisc	0.0015388	Pa×s	466.60	Joback Method
dvisc	0.0005130	Pa×s	683.14	Joback Method
dvisc	0.0005854	Pa×s	647.05	Joback Method
dvisc	0.0006785	Pa×s	610.96	Joback Method
dvisc	0.0008012	Pa×s	574.87	Joback Method
dvisc	0.0009673	Pa×s	538.78	Joback Method
dvisc	0.0011999	Pa×s	502.69	Joback Method
hfust	27.10	kJ/mol	431.60	NIST Webbook
hsubt	106.20	kJ/mol	340.00	NIST Webbook
hsubt	106.20 ± 1.10	kJ/mol	358.00	NIST Webbook
hsubt	107.20 ± 0.80	kJ/mol	358.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29446159&Units=SI
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

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

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