

Dibenzo[b,e][1,4]dioxin, 2,8-dichloro-

Other names:	2,8-Dichlorodibenzo-p-dioxin Dibenzo-p-dioxin, 2,8-dichloro
Inchi:	InChI=1S/C12H6Cl2O2/c13-7-1-3-9-11(5-7)16-12-6-8(14)2-4-10(12)15-9/h1-6H
InchiKey:	WMWJCKBJUQDYLM-UHFFFAOYSA-N
Formula:	C12H6Cl2O2
SMILES:	Clc1ccc2c(c1)Oc1cc(Cl)ccc1O2
Mol. weight [g/mol]:	253.08
CAS:	38964-22-6

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
hvap	67.35	kJ/mol	Joback Method
ie	7.80 ± 0.00	eV	NIST Webbook
log10ws	-7.18		Aqueous Solubility Prediction Method
logp	4.891		Crippen Method
mcvol	157.780	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1996.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1976.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1996.00		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	357.63	J/mol×K	683.14	Joback Method
cpg	367.82	J/mol×K	726.84	Joback Method
cpg	377.11	J/mol×K	770.55	Joback Method
cpg	385.63	J/mol×K	814.25	Joback Method
cpg	393.51	J/mol×K	857.96	Joback Method
cpg	400.86	J/mol×K	901.66	Joback Method
cpg	407.80	J/mol×K	945.37	Joback Method
dvisc	0.0015388	Pa×s	466.60	Joback Method
dvisc	0.0011999	Pa×s	502.69	Joback Method
dvisc	0.0009673	Pa×s	538.78	Joback Method
dvisc	0.0008012	Pa×s	574.87	Joback Method
dvisc	0.0006785	Pa×s	610.96	Joback Method
dvisc	0.0005854	Pa×s	647.05	Joback Method
dvisc	0.0005130	Pa×s	683.14	Joback Method
hsubt	109.00	kJ/mol	334.00	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C38964226&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

ie:	Ionization energy
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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