1,2-dichloro dibenzo-p-dioxin

Other names: Dibenzo-p-dioxin, 1,2-dichloro
Inchi: InChI=1S/C12H6Cl2O2/c13-7-5-6-10-12(11(7)14)16-9-4-2-1-3-8(9)15-10/h1-6H
InchiKey: DFGDMWHUCCHXIF-UHFFFAOYSA-N
Formula: C12H6Cl2O2
SMILES: Clc1ccc2c(c1Cl)Oc1ccccc1O2
Mol. weight [g/mol]: 253.08

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
log10ws	-4.36		Crippen Method
logp	4.891		Crippen Method
mcvol	157.780	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	2001.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	2002.00		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	400.86	J/mol×K	901.66	Joback Method
cpg	393.51	J/mol×K	857.96	Joback Method
cpg	385.63	J/mol×K	814.25	Joback Method
cpg	377.11	J/mol×K	770.55	Joback Method
cpg	367.82	J/mol×K	726.84	Joback Method

cpg	407.80	J/mol×K	945.37	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
dvisc	0.0015388	Pa×s	466.60	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R37606&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
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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