Dibenzodioxin, 1,6-dibromo-, 3,8-dichloro-

Other names: 1,6-dibromo-3,8-dichloro-dibenzo-p-dioxin
Inchi: InChI=1S/C12H4Br2Cl2O2/c13-7-1-5(15)3-9-11(7)17-10-4-6(16)2-8(14)12(10)18-9/h1-4H
InchiKey: ONFKSSOQJGAEGN-UHFFFAOYSA-N
Formula: C12H4Br2Cl2O2
SMILES: Clc1cc(Br)c2c(c1)Oc1c(Br)cc(Cl)cc1O2
Mol. weight [g/mol]: 410.87

Physical Properties

Property code	Value	Unit	Source
gf	130.30	kJ/mol	Joback Method
hf	-30.29	kJ/mol	Joback Method
hfus	46.67	kJ/mol	Joback Method
hvap	81.54	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	6.416		Crippen Method
mcvol	192.780	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
rinpol	2471.00		NIST Webbook
rinpol	2471.00		NIST Webbook
rinpol	2474.00		NIST Webbook
rinpol	2471.00		NIST Webbook
tb	825.42	K	Joback Method
tc	1108.05	K	Joback Method
tf	611.24	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.92	J/mol×K	825.42	Joback Method
cpg	409.40	J/mol×K	872.53	Joback Method
cpg	416.49	J/mol×K	919.63	Joback Method
cpg	423.35	J/mol×K	966.74	Joback Method
cpg	430.15	J/mol×K	1013.84	Joback Method

cpg	437.04	J/mol×K	1060.95	Joback Method
cpg	444.20	J/mol×K	1108.05	Joback Method
dvisc	0.0010117	Pa×s	611.24	Joback Method
dvisc	0.0008382	Pa×s	646.94	Joback Method
dvisc	0.0007082	Pa×s	682.63	Joback Method
dvisc	0.0006085	Pa×s	718.33	Joback Method
dvisc	0.0005304	Pa×s	754.03	Joback Method
dvisc	0.0004681	Pa×s	789.72	Joback Method
dvisc	0.0004177	Pa×s	825.42	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R171450&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
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