Dibenzodioxin, 1,6-dibromo-, 2,7-dichloro-

Other names: 1,6-dibromo,2,7-dichloro-dibenzo-dioxin
Inchi: InChI=1S/C12H4Br2Cl2O2/c13-9-5(15)1-3-7-11(9)18-8-4-2-6(16)10(14)12(8)17-7/h1-4H
InchiKey: KVYOLMAQQRVDCL-UHFFFAOYSA-N
Formula: C12H4Br2Cl2O2
SMILES: Clc1ccc2c(c1Br)Oc1ccc(Cl)c(Br)c1O2
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	2584.00		NIST Webbook
rinpol	2584.00		NIST Webbook
rinpol	2584.00		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	437.04	J/mol×K	1060.95	Joback Method
cpg	430.15	J/mol×K	1013.84	Joback Method
cpg	423.35	J/mol×K	966.74	Joback Method
cpg	416.49	J/mol×K	919.63	Joback Method
cpg	409.40	J/mol×K	872.53	Joback Method

cpg	444.20	J/mol×K	1108.05	Joback Method
dvisc	0.0004177	Pa×s	825.42	Joback Method
dvisc	0.0004681	Pa×s	789.72	Joback Method
dvisc	0.0005304	Pa×s	754.03	Joback Method
dvisc	0.0006085	Pa×s	718.33	Joback Method
dvisc	0.0007082	Pa×s	682.63	Joback Method
dvisc	0.0008382	Pa×s	646.94	Joback Method
dvisc	0.0010117	Pa×s	611.24	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=R172557&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

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