Dibenzodioxin, 3,7,9-tribromo-, 1,2,6-trichloro-

Other names: 3,7,9-tribromo-1,2,6-trichloro-dibenzo-p-dioxin
Inchi: InChI=1S/C12H2Br3Cl3O2/c13-3-1-5(15)10-12(8(3)17)19-6-2-4(14)7(16)9(18)11(6)20-10
InchiKey: PSWRUKBLFZULLY-UHFFFAOYSA-N
Formula: C12H2Br3Cl3O2
SMILES: Clc1c(Br)cc2c(c1Cl)Oc1c(Br)cc(Br)c(Cl)c1O2
Mol. weight [g/mol]: 524.21

Physical Properties

Property code	Value	Unit	Source
gf	113.43	kJ/mol	Joback Method
hf	-42.64	kJ/mol	Joback Method
hfus	55.37	kJ/mol	Joback Method
hvap	93.68	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	7.832		Crippen Method
mcvol	222.520	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
rinpol	3067.00		NIST Webbook
rinpol	3067.00		NIST Webbook
rinpol	3067.00		NIST Webbook
tb	938.97	K	Joback Method
tc	1230.73	K	Joback Method
tf	726.00	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.25	J/mol×K	938.97	Joback Method
cpg	466.58	J/mol×K	1182.11	Joback Method
cpg	458.59	J/mol×K	1133.48	Joback Method
cpg	451.24	J/mol×K	1084.85	Joback Method
cpg	444.35	J/mol×K	1036.22	Joback Method
cpg	437.74	J/mol×K	987.60	Joback Method

cpg	475.38	J/mol×K	1230.73	Joback Method
dvisc	0.0003066	Pa×s	938.97	Joback Method
dvisc	0.0003395	Pa×s	903.48	Joback Method
dvisc	0.0003791	Pa×s	867.98	Joback Method
dvisc	0.0004273	Pa×s	832.49	Joback Method
dvisc	0.0004869	Pa×s	796.99	Joback Method
dvisc	0.0005615	Pa×s	761.50	Joback Method
dvisc	0.0006566	Pa×s	726.00	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=R172106&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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