2,3,7,8-tetrabromo-1,9-dichloro-dibenzo-p-dioxin

Other names: Dibenzodioxin, 2,3,7,8-tetrabromo-, 1,9-dichloro-
Inchi: InChI=1S/C12H2Br4Cl2O2/c13-3-1-5-11(9(17)7(3)15)20-12-6(19-5)2-4(14)8(16)10(12)18
InchiKey: QHXTVCCFAGTTBW-UHFFFAOYSA-N
Formula: C12H2Br4Cl2O2
SMILES: Clc1c(Br)c(Br)cc2c1Oc1c(cc(Br)c(Br)c1Cl)O2
Mol. weight [g/mol]: 568.66

Physical Properties

Property code	Value	Unit	Source
gf	139.68	kJ/mol	Joback Method
hf	-0.57	kJ/mol	Joback Method
hfus	56.46	kJ/mol	Joback Method
hvap	95.73	kJ/mol	Joback Method
log10ws	-9.01		Crippen Method
logp	7.941		Crippen Method
mcvol	227.780	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
rinpol	3282.00		NIST Webbook
rinpol	3282.00		NIST Webbook
rinpol	3282.00		NIST Webbook
tb	967.70	K	Joback Method
tc	1266.25	K	Joback Method
tf	755.88	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.76	J/mol×K	967.70	Joback Method
cpg	442.66	J/mol×K	1017.46	Joback Method
cpg	449.93	J/mol×K	1067.22	Joback Method
cpg	457.76	J/mol×K	1116.97	Joback Method
cpg	466.35	J/mol×K	1166.73	Joback Method
cpg	475.92	J/mol×K	1216.49	Joback Method

cpg	486.67	J/mol×K	1266.25	Joback Method
dvisc	0.0005793	Pa×s	755.88	Joback Method
dvisc	0.0004983	Pa×s	791.18	Joback Method
dvisc	0.0004342	Pa×s	826.49	Joback Method
dvisc	0.0003826	Pa×s	861.79	Joback Method
dvisc	0.0003405	Pa×s	897.09	Joback Method
dvisc	0.0003058	Pa×s	932.40	Joback Method
dvisc	0.0002767	Pa×s	967.70	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=R171732&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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