1,9-dibromo-2,3,6,7-tetrachloro-dibenzo-p-dioxin

Other names: Dibenzodioxin, 1,9-dibromo-, 2,3,6,7-tetrachloro-
Inchi: InChI=1S/C12H2Br2Cl4O2/c13-3-1-4(15)9(18)12-10(3)20-11-6(19-12)2-5(16)8(17)7(11)1
InchiKey: QNLYQAJISQSROV-UHFFFAOYSA-N
Formula: C12H2Br2Cl4O2
SMILES: Clc1cc2c(c(Br)c1Cl)Oc1c(Br)cc(Cl)c(Cl)c1O2
Mol. weight [g/mol]: 479.76

Physical Properties

Property code	Value	Unit	Source
gf	87.18	kJ/mol	Joback Method
hf	-84.71	kJ/mol	Joback Method
hfus	54.29	kJ/mol	Joback Method
hvap	91.63	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	7.723		Crippen Method
mcvol	217.260	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	2940.00		NIST Webbook
rinpol	2940.00		NIST Webbook
rinpol	2940.00		NIST Webbook
tb	910.24	K	Joback Method
tc	1195.12	K	Joback Method
tf	696.12	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.85	J/mol×K	910.24	Joback Method
cpg	433.11	J/mol×K	957.72	Joback Method
cpg	439.29	J/mol×K	1005.20	Joback Method
cpg	445.52	J/mol×K	1052.68	Joback Method
cpg	451.96	J/mol×K	1100.16	Joback Method
cpg	458.74	J/mol×K	1147.64	Joback Method

cpg	466.02	J/mol×K	1195.12	Joback Method
dvisc	0.0007377	Pa×s	696.12	Joback Method
dvisc	0.0006269	Pa×s	731.81	Joback Method
dvisc	0.0005408	Pa×s	767.49	Joback Method
dvisc	0.0004727	Pa×s	803.18	Joback Method
dvisc	0.0004180	Pa×s	838.87	Joback Method
dvisc	0.0003733	Pa×s	874.55	Joback Method
dvisc	0.0003364	Pa×s	910.24	Joback Method

Sources

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=R171490&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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