2,3,7-tribromo-1,9-dichloro-dibenzo-p-dioxin

Other names: Dibenzodioxin, 2,3,7-tribromo-, 1,9-dichloro-
Inchi: InChI=1S/C12H3Br3Cl2O2/c13-4-1-6(16)11-7(2-4)18-8-3-5(14)9(15)10(17)12(8)19-11/h1
InchiKey: DGXRAKTXYXNSEN-UHFFFAOYSA-N
Formula: C12H3Br3Cl2O2
SMILES: Clc1cc(Br)cc2c1Oc1c(cc(Br)c(Br)c1Cl)O2
Mol. weight [g/mol]: 489.77

Physical Properties

Property code	Value	Unit	Source
gf	134.99	kJ/mol	Joback Method
hf	-15.43	kJ/mol	Joback Method
hfus	51.57	kJ/mol	Joback Method
hvap	88.64	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	7.179		Crippen Method
mcvol	210.280	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
rinpol	2875.00		NIST Webbook
rinpol	2875.00		NIST Webbook
tb	896.56	K	Joback Method
tc	1187.57	K	Joback Method
tf	683.56	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.58	J/mol×K	896.56	Joback Method
cpg	426.45	J/mol×K	945.06	Joback Method
cpg	433.27	J/mol×K	993.56	Joback Method
cpg	440.23	J/mol×K	1042.06	Joback Method
cpg	447.51	J/mol×K	1090.57	Joback Method
cpg	455.30	J/mol×K	1139.07	Joback Method
cpg	463.77	J/mol×K	1187.57	Joback Method

dvisc	0.0007743	Pa×s	683.56	Joback Method
dvisc	0.0006549	Pa×s	719.06	Joback Method
dvisc	0.0005628	Pa×s	754.56	Joback Method
dvisc	0.0004902	Pa×s	790.06	Joback Method
dvisc	0.0004321	Pa×s	825.56	Joback Method
dvisc	0.0003849	Pa×s	861.06	Joback Method
dvisc	0.0003460	Pa×s	896.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R171752&Units=SI
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

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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