1-bromo,2,4,6,7,9-pentachloro-dibenzo-dioxin

Inchi: InChI=1S/C12H2BrCl5O2/c13-7-3(14)1-5(16)9-11(7)19-10-6(17)2-4(15)8(18)12(10)20-9/
InchiKey: JYBLMFICMILPCH-UHFFFAOYSA-N
Formula: C12H2BrCl5O2
SMILES: Clc1cc(Cl)c2c(c1Cl)Oc1c(Cl)cc(Cl)c(Br)c1O2
Mol. weight [g/mol]: 435.31

Physical Properties

Property code	Value	Unit	Source
gf	60.93	kJ/mol	Joback Method
hf	-126.78	kJ/mol	Joback Method
hfus	53.20	kJ/mol	Joback Method
hvap	89.58	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	7.614		Crippen Method
mcvol	212.000	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	2772.00		NIST Webbook
rinpol	2772.00		NIST Webbook
tb	881.51	K	Joback Method
tc	1159.42	K	Joback Method
tf	666.24	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.41	J/mol×K	881.51	Joback Method
cpg	428.61	J/mol×K	927.83	Joback Method
cpg	434.56	J/mol×K	974.15	Joback Method
cpg	440.37	J/mol×K	1020.46	Joback Method
cpg	446.17	J/mol×K	1066.78	Joback Method
cpg	452.08	J/mol×K	1113.10	Joback Method
cpg	458.23	J/mol×K	1159.42	Joback Method
dvisc	0.0008204	Pa×s	666.24	Joback Method

dvisc	0.0006924	Pa×s	702.12	Joback Method
dvisc	0.0005942	Pa×s	738.00	Joback Method
dvisc	0.0005171	Pa×s	773.88	Joback Method
dvisc	0.0004556	Pa×s	809.75	Joback Method
dvisc	0.0004058	Pa×s	845.63	Joback Method
dvisc	0.0003648	Pa×s	881.51	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=R172646&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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