2-bromo,1,3,4,6,7,8,9-heptachloro-dibenzo-dioxin

Inchi: InChI=1S/C12BrCl7O2/c13-1-2(14)6(18)10-9(3(1)15)21-11-7(19)4(16)5(17)8(20)12(11)22
InchiKey: QWQSAEFEFCNQDW-UHFFFAOYSA-N
Formula: C12BrCl7O2
SMILES: Clc1c(Cl)c(Cl)c2c(c1Cl)Oc1c(Cl)c(Cl)c(Br)c(Cl)c1O2
Mol. weight [g/mol]: 504.20

Physical Properties

Property code	Value	Unit	Source
gf	17.81	kJ/mol	Joback Method
hf	-181.20	kJ/mol	Joback Method
hfus	60.81	kJ/mol	Joback Method
hvap	99.68	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	8.921		Crippen Method
mcvol	236.480	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	3243.00		NIST Webbook
tb	966.33	K	Joback Method
tc	1246.90	K	Joback Method
tf	751.12	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.50	J/mol×K	966.33	Joback Method
cpg	449.72	J/mol×K	1013.09	Joback Method
cpg	454.89	J/mol×K	1059.85	Joback Method
cpg	460.13	J/mol×K	1106.61	Joback Method
cpg	465.52	J/mol×K	1153.38	Joback Method
cpg	471.18	J/mol×K	1200.14	Joback Method
cpg	477.22	J/mol×K	1246.90	Joback Method
dvisc	0.0006027	Pa×s	751.12	Joback Method
dvisc	0.0005194	Pa×s	786.99	Joback Method

dvisc	0.0004535	Pa×s	822.86	Joback Method
dvisc	0.0004004	Pa×s	858.73	Joback Method
dvisc	0.0003571	Pa×s	894.59	Joback Method
dvisc	0.0003213	Pa×s	930.46	Joback Method
dvisc	0.0002914	Pa×s	966.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172775&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