2-bromo,1,6,9-trichloro-dibenzo-dioxin

Inchi: InChI=1S/C12H4BrCl3O2/c13-5-1-4-8-12(9(5)16)18-11-7(15)3-2-6(14)10(11)17-8/h1-4H
InchiKey: OKMWETQDHUKKRF-UHFFFAOYSA-N
Formula: C12H4BrCl3O2
SMILES: Clc1ccc(Cl)c2c1Oc1ccc(Br)c(Cl)c1O2
Mol. weight [g/mol]: 366.42

Physical Properties

Property code	Value	Unit	Source
gf	104.05	kJ/mol	Joback Method
hf	-72.36	kJ/mol	Joback Method
hfus	45.58	kJ/mol	Joback Method
hvap	79.49	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	6.307		Crippen Method
mcvol	187.520	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	2461.00		NIST Webbook
rinpol	2461.00		NIST Webbook
tb	796.69	K	Joback Method
tc	1071.66	K	Joback Method
tf	581.36	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.46	J/mol×K	796.69	Joback Method
cpg	404.13	J/mol×K	842.52	Joback Method
cpg	411.28	J/mol×K	888.35	Joback Method
cpg	418.04	J/mol×K	934.17	Joback Method
cpg	424.55	J/mol×K	980.00	Joback Method
cpg	430.95	J/mol×K	1025.83	Joback Method
cpg	437.37	J/mol×K	1071.66	Joback Method
dvisc	0.0011065	Pa×s	581.36	Joback Method

dvisc	0.0009086	Pa×s	617.25	Joback Method
dvisc	0.0007624	Pa×s	653.14	Joback Method
dvisc	0.0006515	Pa×s	689.03	Joback Method
dvisc	0.0005655	Pa×s	724.91	Joback Method
dvisc	0.0004974	Pa×s	760.80	Joback Method
dvisc	0.0004427	Pa×s	796.69	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=R172819&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