2,3,7-tribromo,1-chloro-dibenzo-dioxin

Inchi: InChI=1S/C12H4Br3ClO2/c13-5-1-2-7-8(3-5)17-9-4-6(14)10(15)11(16)12(9)18-7/h1-4H
InchiKey: OJBITULZKGPLND-UHFFFAOYSA-N
Formula: C12H4Br3ClO2
SMILES: Clc1c(Br)c(Br)cc2c1Oc1ccc(Br)cc1O2
Mol. weight [g/mol]: 455.32

Physical Properties

Property code	Value	Unit	Source
gf	156.55	kJ/mol	Joback Method
hf	11.78	kJ/mol	Joback Method
hfus	47.76	kJ/mol	Joback Method
hvap	83.59	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.526		Crippen Method
mcvol	198.040	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
rinpol	2707.00		NIST Webbook
rinpol	2707.00		NIST Webbook
tb	854.15	K	Joback Method
tc	1144.33	K	Joback Method
tf	641.12	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.09	J/mol×K	854.15	Joback Method
cpg	414.50	J/mol×K	902.51	Joback Method
cpg	421.68	J/mol×K	950.88	Joback Method
cpg	428.84	J/mol×K	999.24	Joback Method
cpg	436.15	J/mol×K	1047.60	Joback Method
cpg	443.83	J/mol×K	1095.96	Joback Method
cpg	452.05	J/mol×K	1144.33	Joback Method
dvisc	0.0009125	Pa×s	641.12	Joback Method

dvisc	0.0007623	Pa×s	676.62	Joback Method
dvisc	0.0006483	Pa×s	712.13	Joback Method
dvisc	0.0005599	Pa×s	747.63	Joback Method
dvisc	0.0004901	Pa×s	783.14	Joback Method
dvisc	0.0004339	Pa×s	818.64	Joback Method
dvisc	0.0003881	Pa×s	854.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172700&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

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