Phenol, 2,2'-methylenebis(3,5,6-trichloro-

Other names: 2,2'-Methylenebis(3,5,6-trichlorophenol)
Inchi: InChI=1S/C13H6Cl6O2/c14-6-2-8(16)10(18)12(20)4(6)1-5-7(15)3-9(17)11(19)13(5)21/h2
InchiKey: SPFVBVIRMDLUJI-UHFFFAOYSA-N
Formula: C13H4Cl6O2
SMILES: Oc1c(Cl)c(Cl)cc(Cl)c1Cc1c(Cl)cc(Cl)c(Cl)c1O
Mol. weight [g/mol]: 404.89
CAS: 19386-45-9

Physical Properties

Property code	Value	Unit	Source
gf	-155.20	kJ/mol	Joback Method
hf	-356.47	kJ/mol	Joback Method
hfus	51.92	kJ/mol	Joback Method
hvap	105.39	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	6.609		Crippen Method
mcvol	231.690	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
tb	965.90	K	Joback Method
tc	1239.16	K	Joback Method
tf	767.19	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.06	J/mol×K	965.90	Joback Method
cpg	531.63	J/mol×K	1011.44	Joback Method
cpg	541.74	J/mol×K	1056.99	Joback Method
cpg	552.60	J/mol×K	1102.53	Joback Method
cpg	564.41	J/mol×K	1148.07	Joback Method
cpg	577.38	J/mol×K	1193.62	Joback Method
cpg	591.71	J/mol×K	1239.16	Joback Method
dvisc	0.0000012	Pa×s	767.19	Joback Method

dvisc	0.0000008	Pa×s	800.31	Joback Method
dvisc	0.0000006	Pa×s	833.43	Joback Method
dvisc	0.0000004	Pa×s	866.55	Joback Method
dvisc	0.0000003	Pa×s	899.66	Joback Method
dvisc	0.0000002	Pa×s	932.78	Joback Method
dvisc	0.0000002	Pa×s	965.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19386459&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume