2,5-Dichloro-3,4,6-tris[(2,2-dichloropropanoyl)oxy 2,2-dichloropropanoate

Inchi: InChI=1S/C18H12Cl10O8/c1-15(21,22)11(29)33-7-5(19)9(35-13(31)17(3,25)26)10(36-14
InchiKey: ORHLVVMKMXLUHL-UHFFFAOYSA-N
Formula: C18H12Cl10O8
SMILES: CC(Cl)(Cl)C(=O)Oc1c(Cl)c(OC(=O)C(C)(Cl)Cl)c(OC(=O)C(C)(Cl)Cl)c(Cl)c1OC(=O)C(C)(
Mol. weight [g/mol]: 710.81
CAS: 109593-91-1

Physical Properties

Property code	Value	Unit	Source
gf	-878.68	kJ/mol	Joback Method
hf	-1407.27	kJ/mol	Joback Method
hfus	57.93	kJ/mol	Joback Method
hvap	136.54	kJ/mol	Joback Method
log10ws	-9.42		Crippen Method
logp	7.390		Crippen Method
mcvol	392.880	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
tb	1329.36	K	Joback Method
tc	1627.74	K	Joback Method
tf	979.16	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	961.18	J/mol×K	1329.36	Joback Method
cpg	961.96	J/mol×K	1379.09	Joback Method
cpg	962.32	J/mol×K	1428.82	Joback Method
cpg	962.40	J/mol×K	1478.55	Joback Method
cpg	962.39	J/mol×K	1528.28	Joback Method
cpg	962.44	J/mol×K	1578.01	Joback Method
cpg	962.73	J/mol×K	1627.74	Joback Method
dvisc	0.0000072	Pa×s	979.16	Joback Method
dvisc	0.0000051	Pa×s	1037.53	Joback Method

dvisc	0.0000038	Pa×s	1095.89	Joback Method
dvisc	0.0000029	Pa×s	1154.26	Joback Method
dvisc	0.0000022	Pa×s	1212.63	Joback Method
dvisc	0.0000018	Pa×s	1270.99	Joback Method
dvisc	0.0000015	Pa×s	1329.36	Joback Method

Sources

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=C109593911&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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