3,5-Dichloro-2-[(2,2-dichloropropanoyl)oxy]benzyl 2,2-dichloropropanoate

Inchi: InChI=1S/C13H10Cl6O4/c1-12(16,17)10(20)22-5-6-3-7(14)4-8(15)9(6)23-11(21)13(2,18)19/h3-4H,5H2,1-2H3

InchiKey: GTQBBVDDVNXYOT-UHFFFAOYSA-N

Formula: C13H10Cl6O4

SMILES: CC(Cl)(Cl)C(=O)OCc1cc(Cl)cc(Cl)c1OC(=O)C(C)(Cl)Cl

Mol. weight [g/mol]: 442.93

CAS: 108878-18-8

Physical Properties

Property code	Value	Unit	Source
gf	-391.64	kJ/mol	Joback Method
hf	-711.07	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	90.82	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.330		Crippen Method
mcvol	258.590	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
tb	909.16	K	Joback Method
tc	1156.84	K	Joback Method
tf	628.93	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.84	J/mol×K	909.16	Joback Method
cpg	622.22	J/mol×K	950.44	Joback Method
cpg	628.75	J/mol×K	991.72	Joback Method
cpg	634.49	J/mol×K	1033.00	Joback Method
cpg	639.51	J/mol×K	1074.28	Joback Method
cpg	643.89	J/mol×K	1115.56	Joback Method
cpg	647.69	J/mol×K	1156.84	Joback Method
dvisc	0.0002194	Pa×s	628.93	Joback Method
dvisc	0.0001467	Pa×s	675.64	Joback Method

dvisc	0.0001034	Pa×s	722.34	Joback Method
dvisc	0.0000760	Pa×s	769.05	Joback Method
dvisc	0.0000579	Pa×s	815.75	Joback Method
dvisc	0.0000454	Pa×s	862.46	Joback Method
dvisc	0.0000365	Pa×s	909.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108878188&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume