

3-[(2,2-Dichloropropanoyl)oxy]-2,2-bis([(2,2-dichloropropanoyl)oxy]oxy)propane

InChI: InChI=1S/C17H20Cl8O8/c1-13(18,19)9(26)30-5-17(6-31-10(27)14(2,20)21,7-32-11(28)15

InchiKey: WOKUVVRQHMYMGQ-UHFFFAOYSA-N

Formula: C17H20Cl8O8

SMILES: CC(Cl)(Cl)C(=O)OCC(COC(=O)C(C)(Cl)Cl)(COC(=O)C(C)(Cl)Cl)COC(=O)C(C)(Cl)Cl

Mol. weight [g/mol]: 635.96

CAS: 116295-67-1

Physical Properties

Property code	Value	Unit	Source
gf	-924.66	kJ/mol	Joback Method
hf	-1543.08	kJ/mol	Joback Method
hfus	47.44	kJ/mol	Joback Method
hvap	118.66	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.921		Crippen Method
mcvol	378.070	ml/mol	McGowan Method
pc	1216.59	kPa	Joback Method
tb	1176.81	K	Joback Method
tc	1441.08	K	Joback Method
tf	821.45	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.26	J/molxK	1176.81	Joback Method
cpg	1040.03	J/molxK	1220.86	Joback Method
cpg	1046.57	J/molxK	1264.90	Joback Method
cpg	1053.07	J/molxK	1308.95	Joback Method
cpg	1059.72	J/molxK	1352.99	Joback Method
cpg	1066.70	J/molxK	1397.04	Joback Method
cpg	1074.21	J/molxK	1441.08	Joback Method
dvisc	0.0000153	Paxs	821.45	Joback Method
dvisc	0.0000094	Paxs	880.68	Joback Method

dvisc	0.0000061	Paxs	939.90	Joback Method
dvisc	0.0000042	Paxs	999.13	Joback Method
dvisc	0.0000030	Paxs	1058.36	Joback Method
dvisc	0.0000022	Paxs	1117.58	Joback Method
dvisc	0.0000017	Paxs	1176.81	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C116295671&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/79-935-7/3-2-2-Dichloropropanoyl-oxy-2-2-bis-2-2-dichloropropanoyl-oxy-methyl-propyl>

Generated by Cheméo on 2024-04-26 08:45:23.137491189 +0000 UTC m=+16410372.058068509.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.