Diglycolic acid, 2,3-dichlorophenyl heptyl ester

Inchi: InChI=1S/C17H22Cl2O5/c1-2-3-4-5-6-10-23-15(20)11-22-12-16(21)24-14-9-7-8-13(18)17

InchiKey: NWQZTHMKGOTFAA-UHFFFAOYSA-N

Formula: C17H22Cl2O5

SMILES: CCCCCCCOC(=O)COCC(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 377.26

Physical Properties

Property code	Value	Unit	Source
gf	-411.29	kJ/mol	Joback Method
hf	-833.92	kJ/mol	Joback Method
hfus	48.20	kJ/mol	Joback Method
hvap	86.53	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.429		Crippen Method
mcvol	271.860	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	3193.00		NIST Webbook
rinpol	3193.00		NIST Webbook
tb	874.86	K	Joback Method
tc	1084.98	K	Joback Method
tf	559.20	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.22	J/mol×K	874.86	Joback Method
cpg	794.77	J/mol×K	909.88	Joback Method
cpg	806.18	J/mol×K	944.90	Joback Method
cpg	816.46	J/mol×K	979.92	Joback Method
cpg	825.61	J/mol×K	1014.94	Joback Method
cpg	833.63	J/mol×K	1049.96	Joback Method
cpg	840.51	J/mol×K	1084.98	Joback Method
dvisc	0.0003376	Pa×s	559.20	Joback Method

dvisc	0.0002114	Pa×s	611.81	Joback Method
dvisc	0.0001426	Pa×s	664.42	Joback Method
dvisc	0.0001019	Pa×s	717.03	Joback Method
dvisc	0.0000762	Pa×s	769.64	Joback Method
dvisc	0.0000592	Pa×s	822.25	Joback Method
dvisc	0.0000474	Pa×s	874.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382094&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume