Diglycolic acid, 2,6-dichlorophenyl pentyl ester

Inchi: InChI=1S/C15H18Cl2O5/c1-2-3-4-8-21-13(18)9-20-10-14(19)22-15-11(16)6-5-7-12(15)17

InchiKey: RQLUHGKIMHFAAQ-UHFFFAOYSA-N

Formula: C15H18Cl2O5

SMILES: CCCCCOC(=O)COCC(=O)Oc1c(Cl)cccc1Cl

Mol. weight [g/mol]: 349.21

Physical Properties

Property code	Value	Unit	Source
gf	-428.13	kJ/mol	Joback Method
hf	-792.64	kJ/mol	Joback Method
hfus	43.02	kJ/mol	Joback Method
hvap	82.08	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.649		Crippen Method
mcvol	243.680	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	2861.00		NIST Webbook
rinpol	2861.00		NIST Webbook
tb	829.10	K	Joback Method
tc	1040.04	K	Joback Method
tf	536.66	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.63	J/mol×K	829.10	Joback Method
cpg	681.71	J/mol×K	864.26	Joback Method
cpg	692.77	J/mol×K	899.41	Joback Method
cpg	702.79	J/mol×K	934.57	Joback Method
cpg	711.77	J/mol×K	969.73	Joback Method
cpg	719.71	J/mol×K	1004.89	Joback Method
cpg	726.60	J/mol×K	1040.04	Joback Method
dvisc	0.0004117	Pa×s	536.66	Joback Method

dvisc	0.0002643	Pa×s	585.40	Joback Method
dvisc	0.0001817	Pa×s	634.14	Joback Method
dvisc	0.0001318	Pa×s	682.88	Joback Method
dvisc	0.0000997	Pa×s	731.62	Joback Method
dvisc	0.0000782	Pa×s	780.36	Joback Method
dvisc	0.0000630	Pa×s	829.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382299&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume