Diglycolic acid, 4-chlorophenyl isohexyl ester

Inchi: InChI=1S/C16H21ClO5/c1-12(2)4-3-9-21-15(18)10-20-11-16(19)22-14-7-5-13(17)6-8-14/
InchiKey: UQXLZYZFNQECJY-UHFFFAOYSA-N
Formula: C16H21ClO5
SMILES: CC(C)CCCOC(=O)COCC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 328.79

Physical Properties

Property code	Value	Unit	Source
gf	-400.59	kJ/mol	Joback Method
hf	-791.35	kJ/mol	Joback Method
hfus	38.28	kJ/mol	Joback Method
hvap	78.87	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.241		Crippen Method
mcvol	245.530	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	2825.00		NIST Webbook
rinpol	2825.00		NIST Webbook
tb	809.13	K	Joback Method
tc	1016.81	K	Joback Method
tf	490.49	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.05	J/mol×K	809.13	Joback Method
cpg	716.81	J/mol×K	843.74	Joback Method
cpg	729.50	J/mol×K	878.36	Joback Method
cpg	741.11	J/mol×K	912.97	Joback Method
cpg	751.65	J/mol×K	947.58	Joback Method
cpg	761.11	J/mol×K	982.20	Joback Method
cpg	769.51	J/mol×K	1016.81	Joback Method
dvisc	0.0005736	Pa×s	490.49	Joback Method

dvisc	0.0003241	Pa×s	543.60	Joback Method
dvisc	0.0002027	Pa×s	596.70	Joback Method
dvisc	0.0001369	Pa×s	649.81	Joback Method
dvisc	0.0000981	Pa×s	702.92	Joback Method
dvisc	0.0000736	Pa×s	756.02	Joback Method
dvisc	0.0000574	Pa×s	809.13	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=U381780&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume