Diglycolic acid, 4-chlorophenyl hexyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-398.15	kJ/mol	Joback Method
hf	-786.07	kJ/mol	Joback Method
hfus	41.81	kJ/mol	Joback Method
hvap	79.26	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.385		Crippen Method
mcvol	245.530	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	2875.00		NIST Webbook
rinpol	2875.00		NIST Webbook
tb	809.57	K	Joback Method
tc	1014.73	K	Joback Method
tf	505.49	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.49	J/mol×K	809.57	Joback Method
cpg	716.09	J/mol×K	843.76	Joback Method
cpg	728.65	J/mol×K	877.96	Joback Method
cpg	740.17	J/mol×K	912.15	Joback Method
cpg	750.66	J/mol×K	946.34	Joback Method
cpg	760.11	J/mol×K	980.54	Joback Method
cpg	768.53	J/mol×K	1014.73	Joback Method
dvisc	0.0005117	Pa×s	505.49	Joback Method

dvisc	0.0003073	Pa×s	556.17	Joback Method
dvisc	0.0002009	Pa×s	606.85	Joback Method
dvisc	0.0001403	Pa×s	657.53	Joback Method
dvisc	0.0001031	Pa×s	708.21	Joback Method
dvisc	0.0000790	Pa×s	758.89	Joback Method
dvisc	0.0000625	Pa×s	809.57	Joback Method

Sources

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=U381781&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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