Diglycolic acid, 4-chloro-2-methylphenyl octyl ester

Inchi: InChI=1S/C19H27ClO5/c1-3-4-5-6-7-8-11-24-18(21)13-23-14-19(22)25-17-10-9-16(20)12

InchiKey: XENGBHNCFPZUIG-UHFFFAOYSA-N

Formula: C19H27ClO5

SMILES: CCCCCCCCOC(=O)COCC(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 370.87

Physical Properties

Property code	Value	Unit	Source
gf	-382.52	kJ/mol	Joback Method
hf	-859.46	kJ/mol	Joback Method
hfus	49.19	kJ/mol	Joback Method
hvap	86.59	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.474		Crippen Method
mcvol	287.800	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	3203.00		NIST Webbook
rinpol	3203.00		NIST Webbook
tb	883.19	K	Joback Method
tc	1089.77	K	Joback Method
tf	551.82	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.66	J/mol×K	883.19	Joback Method
cpg	887.81	J/mol×K	917.62	Joback Method
cpg	900.75	J/mol×K	952.05	Joback Method
cpg	912.48	J/mol×K	986.48	Joback Method
cpg	923.01	J/mol×K	1020.91	Joback Method
cpg	932.35	J/mol×K	1055.34	Joback Method
cpg	940.50	J/mol×K	1089.77	Joback Method
dvisc	0.0003317	Pa×s	551.82	Joback Method

dvisc	0.0002003	Pa×s	607.05	Joback Method
dvisc	0.0001315	Pa×s	662.28	Joback Method
dvisc	0.0000922	Pa×s	717.50	Joback Method
dvisc	0.0000680	Pa×s	772.73	Joback Method
dvisc	0.0000522	Pa×s	827.96	Joback Method
dvisc	0.0000414	Pa×s	883.19	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=U382745&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