Diglycolic acid, 3-chlorophenyl octyl ester

Inchi: InChI=1S/C18H25ClO5/c1-2-3-4-5-6-7-11-23-17(20)13-22-14-18(21)24-16-10-8-9-15(19)
InchiKey: RXZRIKCHJRHIII-UHFFFAOYSA-N
Formula: C18H25ClO5
SMILES: CCCCCCCCOC(=O)COCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 356.84

Physical Properties

Property code	Value	Unit	Source
gf	-381.31	kJ/mol	Joback Method
hf	-827.35	kJ/mol	Joback Method
hfus	46.99	kJ/mol	Joback Method
hvap	83.71	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.166		Crippen Method
mcvol	273.710	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	3116.00		NIST Webbook
rinpol	3116.00		NIST Webbook
tb	855.33	K	Joback Method
tc	1060.14	K	Joback Method
tf	528.03	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.44	J/mol×K	855.33	Joback Method
cpg	875.37	J/mol×K	1026.01	Joback Method
cpg	865.84	J/mol×K	991.87	Joback Method
cpg	855.18	J/mol×K	957.74	Joback Method
cpg	843.41	J/mol×K	923.60	Joback Method
cpg	830.50	J/mol×K	889.47	Joback Method
cpg	883.79	J/mol×K	1060.14	Joback Method
dvisc	0.0000471	Pa×s	855.33	Joback Method

dvisc	0.0000599	Pa×s	800.78	Joback Method
dvisc	0.0000789	Pa×s	746.23	Joback Method
dvisc	0.0001086	Pa×s	691.68	Joback Method
dvisc	0.0001577	Pa×s	637.13	Joback Method
dvisc	0.0002457	Pa×s	582.58	Joback Method
dvisc	0.0004196	Pa×s	528.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381772&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

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

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