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

Inchi: InChI=1S/C18H25ClO5/c1-3-4-5-6-7-10-23-17(20)12-22-13-18(21)24-16-9-8-15(19)11-14

InchiKey: FENJXVXJIMOQQT-UHFFFAOYSA-N

Formula: C18H25ClO5

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

Mol. weight [g/mol]: 356.84

Physical Properties

Property code	Value	Unit	Source
gf	-390.94	kJ/mol	Joback Method
hf	-838.82	kJ/mol	Joback Method
hfus	46.60	kJ/mol	Joback Method
hvap	84.37	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.084		Crippen Method
mcvol	273.710	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	3083.00		NIST Webbook
rinpol	3083.00		NIST Webbook
tb	860.31	K	Joback Method
tc	1065.97	K	Joback Method
tf	540.55	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.46	J/mol×K	860.31	Joback Method
cpg	829.42	J/mol×K	894.59	Joback Method
cpg	842.23	J/mol×K	928.86	Joback Method
cpg	853.90	J/mol×K	963.14	Joback Method
cpg	864.42	J/mol×K	997.42	Joback Method
cpg	873.80	J/mol×K	1031.70	Joback Method
cpg	882.04	J/mol×K	1065.97	Joback Method
dvisc	0.0003673	Pa×s	540.55	Joback Method

dvisc	0.0002245	Pa×s	593.84	Joback Method
dvisc	0.0001488	Pa×s	647.14	Joback Method
dvisc	0.0001050	Pa×s	700.43	Joback Method
dvisc	0.0000778	Pa×s	753.72	Joback Method
dvisc	0.0000600	Pa×s	807.02	Joback Method
dvisc	0.0000478	Pa×s	860.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382744&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