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

Inchi: InChI=1S/C14H17ClO5/c1-3-6-19-13(16)8-18-9-14(17)20-12-5-4-11(15)7-10(12)2/h4-5,7

InchiKey: DSKTUHJJUFQFEB-UHFFFAOYSA-N

Formula: C14H17ClO5

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

Mol. weight [g/mol]: 300.74

Physical Properties

Property code	Value	Unit	Source
gf	-424.62	kJ/mol	Joback Method
hf	-756.26	kJ/mol	Joback Method
hfus	36.24	kJ/mol	Joback Method
hvap	75.47	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.524		Crippen Method
mcvol	217.350	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	2571.00		NIST Webbook
rinpol	2571.00		NIST Webbook
tb	768.79	K	Joback Method
tc	977.57	K	Joback Method
tf	495.47	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.02	J/mol×K	768.79	Joback Method
cpg	646.01	J/mol×K	942.78	Joback Method
cpg	636.93	J/mol×K	907.98	Joback Method
cpg	626.88	J/mol×K	873.18	Joback Method
cpg	615.87	J/mol×K	838.38	Joback Method
cpg	603.91	J/mol×K	803.59	Joback Method
cpg	654.11	J/mol×K	977.57	Joback Method
dvisc	0.0000824	Pa×s	768.79	Joback Method

dvisc	0.0001019	Pa×s	723.24	Joback Method
dvisc	0.0001297	Pa×s	677.68	Joback Method
dvisc	0.0001708	Pa×s	632.13	Joback Method
dvisc	0.0002347	Pa×s	586.58	Joback Method
dvisc	0.0003404	Pa×s	541.02	Joback Method
dvisc	0.0005286	Pa×s	495.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382739&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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