

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.02	J/molxK	768.79	Joback Method
cpg	603.91	J/molxK	803.59	Joback Method
cpg	615.87	J/molxK	838.38	Joback Method
cpg	626.88	J/molxK	873.18	Joback Method
cpg	636.93	J/molxK	907.98	Joback Method
cpg	646.01	J/molxK	942.78	Joback Method
cpg	654.11	J/molxK	977.57	Joback Method
dvisc	0.0005286	Paxs	495.47	Joback Method

dvisc	0.0003404	Paxs	541.02	Joback Method
dvisc	0.0002347	Paxs	586.58	Joback Method
dvisc	0.0001708	Paxs	632.13	Joback Method
dvisc	0.0001297	Paxs	677.68	Joback Method
dvisc	0.0001019	Paxs	723.24	Joback Method
dvisc	0.0000824	Paxs	768.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U382739&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

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