Diglycolic acid, butyl 3-chlorophenyl ester

Inchi: InChI=1S/C14H17ClO5/c1-2-3-7-19-13(16)9-18-10-14(17)20-12-6-4-5-11(15)8-12/h4-6,8
InchiKey: XNCYSPBKPSBEBZ-UHFFFAOYSA-N
Formula: C14H17ClO5
SMILES: CCCCOC(=O)COCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 300.74

Physical Properties

Property code	Value	Unit	Source
gf	-414.99	kJ/mol	Joback Method
hf	-744.79	kJ/mol	Joback Method
hfus	36.63	kJ/mol	Joback Method
hvap	74.80	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.605		Crippen Method
mcvol	217.350	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	2601.00		NIST Webbook
rinpol	2601.00		NIST Webbook
tb	763.81	K	Joback Method
tc	971.80	K	Joback Method
tf	482.95	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.22	J/mol×K	763.81	Joback Method
cpg	647.66	J/mol×K	937.14	Joback Method
cpg	638.48	J/mol×K	902.47	Joback Method
cpg	628.35	J/mol×K	867.81	Joback Method
cpg	617.25	J/mol×K	833.14	Joback Method
cpg	605.21	J/mol×K	798.48	Joback Method
cpg	655.88	J/mol×K	971.80	Joback Method
dvisc	0.0000820	Pa×s	763.81	Joback Method

dvisc	0.0001028	Pa×s	717.00	Joback Method
dvisc	0.0001330	Pa×s	670.19	Joback Method
dvisc	0.0001788	Pa×s	623.38	Joback Method
dvisc	0.0002521	Pa×s	576.57	Joback Method
dvisc	0.0003779	Pa×s	529.76	Joback Method
dvisc	0.0006127	Pa×s	482.95	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=U381767&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