Diglycolic acid, ethyl phenethyl ester

Inchi: InChI=1S/C14H18O5/c1-2-18-13(15)10-17-11-14(16)19-9-8-12-6-4-3-5-7-12/h3-7H,2,8-1
InchiKey: PYBKCWURVFMLAY-UHFFFAOYSA-N
Formula: C14H18O5
SMILES: CCOC(=O)COCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 266.29

Physical Properties

Property code	Value	Unit	Source
gf	-393.43	kJ/mol	Joback Method
hf	-717.58	kJ/mol	Joback Method
hfus	32.82	kJ/mol	Joback Method
hvap	69.76	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.352		Crippen Method
mcvol	205.110	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	2470.00		NIST Webbook
tb	721.40	K	Joback Method
tc	925.03	K	Joback Method
tf	440.51	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.57	J/mol×K	721.40	Joback Method
cpg	581.76	J/mol×K	755.34	Joback Method
cpg	595.02	J/mol×K	789.28	Joback Method
cpg	607.36	J/mol×K	823.22	Joback Method
cpg	618.77	J/mol×K	857.15	Joback Method
cpg	629.25	J/mol×K	891.09	Joback Method
cpg	638.80	J/mol×K	925.03	Joback Method
dvisc	0.0008544	Pa×s	440.51	Joback Method
dvisc	0.0004931	Pa×s	487.32	Joback Method

dvisc	0.0003134	Pa×s	534.14	Joback Method
dvisc	0.0002142	Pa×s	580.95	Joback Method
dvisc	0.0001550	Pa×s	627.77	Joback Method
dvisc	0.0001173	Pa×s	674.59	Joback Method
dvisc	0.0000921	Pa×s	721.40	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=U382155&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