Diglycolic acid, hexyl phenethyl ester

Inchi: InChI=1S/C18H26O5/c1-2-3-4-8-12-22-17(19)14-21-15-18(20)23-13-11-16-9-6-5-7-10-16
InchiKey: PFWMKOFQXJJMDG-UHFFFAOYSA-N
Formula: C18H26O5
SMILES: CCCCCCOC(=O)COCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 322.40

Physical Properties

Property code	Value	Unit	Source
gf	-359.75	kJ/mol	Joback Method
hf	-800.14	kJ/mol	Joback Method
hfus	43.18	kJ/mol	Joback Method
hvap	78.66	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.912		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1550.00	kPa	Joback Method
rinpol	3015.00		NIST Webbook
rinpol	3015.00		NIST Webbook
tb	812.92	K	Joback Method
tc	1012.09	K	Joback Method
tf	485.59	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.76	J/mol×K	812.92	Joback Method
cpg	806.10	J/mol×K	846.11	Joback Method
cpg	820.33	J/mol×K	879.31	Joback Method
cpg	833.48	J/mol×K	912.50	Joback Method
cpg	845.54	J/mol×K	945.70	Joback Method
cpg	856.54	J/mol×K	978.89	Joback Method
cpg	866.47	J/mol×K	1012.09	Joback Method
dvisc	0.0005959	Pa×s	485.59	Joback Method

dvisc	0.0003262	Pa×s	540.14	Joback Method
dvisc	0.0001994	Pa×s	594.70	Joback Method
dvisc	0.0001324	Pa×s	649.25	Joback Method
dvisc	0.0000937	Pa×s	703.81	Joback Method
dvisc	0.0000697	Pa×s	758.37	Joback Method
dvisc	0.0000539	Pa×s	812.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382161&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