Diglycolic acid, nonyl 3-phenylpropyl ester

Inchi: InChI=1S/C22H34O5/c1-2-3-4-5-6-7-11-16-26-21(23)18-25-19-22(24)27-17-12-15-20-13
InchiKey: RIZBDRJTHAZVMB-UHFFFAOYSA-N
Formula: C22H34O5
SMILES: CCCCCCCCCOC(=O)COCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 378.50

Physical Properties

Property code	Value	Unit	Source
gf	-326.07	kJ/mol	Joback Method
hf	-882.70	kJ/mol	Joback Method
hfus	53.54	kJ/mol	Joback Method
hvap	87.56	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.473		Crippen Method
mcvol	317.830	ml/mol	McGowan Method
pc	1169.62	kPa	Joback Method
rinpol	3500.00		NIST Webbook
rinpol	3500.00		NIST Webbook
tb	904.44	K	Joback Method
tc	1109.57	K	Joback Method
tf	530.67	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.65	J/mol×K	904.44	Joback Method
cpg	1095.08	J/mol×K	1075.38	Joback Method
cpg	1084.17	J/mol×K	1041.19	Joback Method
cpg	1072.00	J/mol×K	1007.01	Joback Method
cpg	1058.53	J/mol×K	972.82	Joback Method
cpg	1043.76	J/mol×K	938.63	Joback Method
cpg	1104.75	J/mol×K	1109.57	Joback Method
dvisc	0.0000302	Pa×s	904.44	Joback Method

dvisc	0.0000395	Pa×s	842.14	Joback Method
dvisc	0.0000538	Pa×s	779.85	Joback Method
dvisc	0.0000775	Pa×s	717.55	Joback Method
dvisc	0.0001196	Pa×s	655.26	Joback Method
dvisc	0.0002022	Pa×s	592.96	Joback Method
dvisc	0.0003866	Pa×s	530.67	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=U382178&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