Diglycolic acid, 3-phenylpropyl propyl ester

Inchi: InChI=1S/C16H22O5/c1-2-10-20-15(17)12-19-13-16(18)21-11-6-9-14-7-4-3-5-8-14/h3-5,
InchiKey: BTHGVXMPAVDFEP-UHFFFAOYSA-N
Formula: C16H22O5
SMILES: CCCOC(=O)COCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 294.34

Physical Properties

Property code	Value	Unit	Source
gf	-376.59	kJ/mol	Joback Method
hf	-758.86	kJ/mol	Joback Method
hfus	38.00	kJ/mol	Joback Method
hvap	74.21	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.132		Crippen Method
mcvol	233.290	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2722.00		NIST Webbook
rinpol	2722.00		NIST Webbook
tb	767.16	K	Joback Method
tc	967.46	K	Joback Method
tf	463.05	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.14	J/mol×K	767.16	Joback Method
cpg	691.99	J/mol×K	800.54	Joback Method
cpg	705.82	J/mol×K	833.93	Joback Method
cpg	718.66	J/mol×K	867.31	Joback Method
cpg	730.48	J/mol×K	900.69	Joback Method
cpg	741.32	J/mol×K	934.07	Joback Method
cpg	751.15	J/mol×K	967.46	Joback Method
dvisc	0.0007211	Pa×s	463.05	Joback Method

dvisc	0.0004049	Pa×s	513.73	Joback Method
dvisc	0.0002521	Pa×s	564.42	Joback Method
dvisc	0.0001698	Pa×s	615.11	Joback Method
dvisc	0.0001214	Pa×s	665.79	Joback Method
dvisc	0.0000910	Pa×s	716.47	Joback Method
dvisc	0.0000709	Pa×s	767.16	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=U382170&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