Diglycolic acid, 3-methylphenyl pentyl ester

Inchi: InChI=1S/C16H22O5/c1-3-4-5-9-20-15(17)11-19-12-16(18)21-14-8-6-7-13(2)10-14/h6-8,
InchiKey: GIWCYMIPISQFSG-UHFFFAOYSA-N
Formula: C16H22O5
SMILES: CCCCCOC(=O)COCC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]: 294.34

Physical Properties

Property code	Value	Unit	Source
gf	-386.22	kJ/mol	Joback Method
hf	-770.33	kJ/mol	Joback Method
hfus	37.61	kJ/mol	Joback Method
hvap	74.87	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.650		Crippen Method
mcvol	233.290	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	2635.00		NIST Webbook
rinpol	2635.00		NIST Webbook
tb	772.14	K	Joback Method
tc	973.24	K	Joback Method
tf	475.57	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.30	J/mol×K	772.14	Joback Method
cpg	691.04	J/mol×K	805.66	Joback Method
cpg	704.79	J/mol×K	839.17	Joback Method
cpg	717.53	J/mol×K	872.69	Joback Method
cpg	729.27	J/mol×K	906.21	Joback Method
cpg	739.99	J/mol×K	939.73	Joback Method
cpg	749.72	J/mol×K	973.24	Joback Method
dvisc	0.0006097	Pa×s	475.57	Joback Method

dvisc	0.0003602	Pa×s	525.00	Joback Method
dvisc	0.0002330	Pa×s	574.43	Joback Method
dvisc	0.0001615	Pa×s	623.86	Joback Method
dvisc	0.0001181	Pa×s	673.28	Joback Method
dvisc	0.0000902	Pa×s	722.71	Joback Method
dvisc	0.0000713	Pa×s	772.14	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=U382101&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