Diglycolic acid, octyl 3-phenylpropyl ester

Inchi: InChI=1S/C21H32O5/c1-2-3-4-5-6-10-15-25-20(22)17-24-18-21(23)26-16-11-14-19-12-8
InchiKey: FEPLBBHBUDRBAJ-UHFFFAOYSA-N
Formula: C21H32O5
SMILES: CCCCCCCCOC(=O)COCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 364.48

Physical Properties

Property code	Value	Unit	Source
gf	-334.49	kJ/mol	Joback Method
hf	-862.06	kJ/mol	Joback Method
hfus	50.95	kJ/mol	Joback Method
hvap	85.34	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.083		Crippen Method
mcvol	303.740	ml/mol	McGowan Method
pc	1250.38	kPa	Joback Method
rinpol	3394.00		NIST Webbook
rinpol	3394.00		NIST Webbook
tb	881.56	K	Joback Method
tc	1084.04	K	Joback Method
tf	519.40	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.40	J/mol×K	881.56	Joback Method
cpg	983.32	J/mol×K	915.31	Joback Method
cpg	997.98	J/mol×K	949.05	Joback Method
cpg	1011.39	J/mol×K	982.80	Joback Method
cpg	1023.57	J/mol×K	1016.55	Joback Method
cpg	1034.55	J/mol×K	1050.29	Joback Method
cpg	1044.34	J/mol×K	1084.04	Joback Method
dvisc	0.0004332	Pa×s	519.40	Joback Method

dvisc	0.0002290	Pa×s	579.76	Joback Method
dvisc	0.0001365	Pa×s	640.12	Joback Method
dvisc	0.0000890	Pa×s	700.48	Joback Method
dvisc	0.0000621	Pa×s	760.84	Joback Method
dvisc	0.0000457	Pa×s	821.20	Joback Method
dvisc	0.0000350	Pa×s	881.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382177&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

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