Diglycolic acid, phenethyl undecyl ester

Inchi: InChI=1S/C23H36O5/c1-2-3-4-5-6-7-8-9-13-17-27-22(24)19-26-20-23(25)28-18-16-21-14
InchiKey: RTDVZTDLJWVXHU-UHFFFAOYSA-N
Formula: C23H36O5
SMILES: CCCCCCCCCCCOC(=O)COCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 392.53

Physical Properties

Property code	Value	Unit	Source
gf	-317.65	kJ/mol	Joback Method
hf	-903.34	kJ/mol	Joback Method
hfus	56.13	kJ/mol	Joback Method
hvap	89.79	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.863		Crippen Method
mcvol	331.920	ml/mol	McGowan Method
pc	1096.44	kPa	Joback Method
rinpol	3641.00		NIST Webbook
rinpol	3641.00		NIST Webbook
tb	927.32	K	Joback Method
tc	1135.98	K	Joback Method
tf	541.94	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.48	J/mol×K	927.32	Joback Method
cpg	1104.78	J/mol×K	962.10	Joback Method
cpg	1119.66	J/mol×K	996.87	Joback Method
cpg	1133.17	J/mol×K	1031.65	Joback Method
cpg	1145.31	J/mol×K	1066.43	Joback Method
cpg	1156.12	J/mol×K	1101.20	Joback Method
cpg	1165.63	J/mol×K	1135.98	Joback Method
dvisc	0.0003438	Pa×s	541.94	Joback Method

dvisc	0.0001780	Pa×s	606.17	Joback Method
dvisc	0.0001045	Pa×s	670.40	Joback Method
dvisc	0.0000674	Pa×s	734.63	Joback Method
dvisc	0.0000466	Pa×s	798.86	Joback Method
dvisc	0.0000340	Pa×s	863.09	Joback Method
dvisc	0.0000260	Pa×s	927.32	Joback Method

Sources

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=U382166&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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