Pimelic acid, 4-methyl-2-pentyl 2-(2-methoxyethyl)hexyl ester

Inchi: InChI=1S/C22H42O5/c1-6-7-11-20(14-15-25-5)17-26-21(23)12-9-8-10-13-22(24)27-19(4
InchiKey: FXRRPNHJXFGQPI-UHFFFAOYSA-N
Formula: C22H42O5
SMILES: CCCCC(CCOC)COC(=O)CCCCCC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 386.57

Physical Properties

Property code	Value	Unit	Source
gf	-445.80	kJ/mol	Joback Method
hf	-1135.07	kJ/mol	Joback Method
hfus	48.93	kJ/mol	Joback Method
hvap	84.12	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	5.301		Crippen Method
mcvol	341.590	ml/mol	McGowan Method
pc	957.91	kPa	Joback Method
rinpol	2422.00		NIST Webbook
rinpol	2422.00		NIST Webbook
tb	876.44	K	Joback Method
tc	1073.13	K	Joback Method
tf	459.25	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.46	J/mol×K	876.44	Joback Method
cpg	1144.31	J/mol×K	909.22	Joback Method
cpg	1161.81	J/mol×K	942.00	Joback Method
cpg	1177.96	J/mol×K	974.78	Joback Method
cpg	1192.79	J/mol×K	1007.57	Joback Method
cpg	1206.30	J/mol×K	1040.35	Joback Method
cpg	1218.52	J/mol×K	1073.13	Joback Method
dvisc	0.0007308	Pa×s	459.25	Joback Method

dvisc	0.0002797	Pa×s	528.78	Joback Method
dvisc	0.0001338	Pa×s	598.31	Joback Method
dvisc	0.0000747	Pa×s	667.85	Joback Method
dvisc	0.0000465	Pa×s	737.38	Joback Method
dvisc	0.0000314	Pa×s	806.91	Joback Method
dvisc	0.0000226	Pa×s	876.44	Joback Method

Sources

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=U406744&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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