Pimelic acid, 4-methyl-2-pentyl 3-(2-methoxyethyl)nonyl ester

Inchi: InChI=1S/C25H48O5/c1-6-7-8-10-13-23(16-18-28-5)17-19-29-24(26)14-11-9-12-15-25(2

InchiKey: GODOBVFMCMSPFZ-UHFFFAOYSA-N

Formula: C25H48O5

SMILES: CCCCCCC(CCOC)CCOC(=O)CCCCCC(=O)OC(C)CC(C)C

Mol. weight [g/mol]: 428.65

Physical Properties

Property code	Value	Unit	Source
gf	-420.54	kJ/mol	Joback Method
hf	-1196.99	kJ/mol	Joback Method
hfus	56.70	kJ/mol	Joback Method
hvap	90.80	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	6.471		Crippen Method
mcvol	383.860	ml/mol	McGowan Method
pc	807.54	kPa	Joback Method
rinpol	2699.00		NIST Webbook
rinpol	2699.00		NIST Webbook
tb	945.08	K	Joback Method
tc	1160.19	K	Joback Method
tf	493.06	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1314.37	J/mol×K	945.08	Joback Method
cpg	1334.34	J/mol×K	980.93	Joback Method
cpg	1352.58	J/mol×K	1016.78	Joback Method
cpg	1369.11	J/mol×K	1052.64	Joback Method
cpg	1383.97	J/mol×K	1088.49	Joback Method
cpg	1397.18	J/mol×K	1124.34	Joback Method
cpg	1408.77	J/mol×K	1160.19	Joback Method
dvisc	0.0004794	Pa×s	493.06	Joback Method

dvisc	0.0001804	Pa×s	568.40	Joback Method
dvisc	0.0000853	Pa×s	643.73	Joback Method
dvisc	0.0000472	Pa×s	719.07	Joback Method
dvisc	0.0000292	Pa×s	794.41	Joback Method
dvisc	0.0000197	Pa×s	869.74	Joback Method
dvisc	0.0000141	Pa×s	945.08	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=U406758&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