Pimelic acid, 4-methyl-2-pentyl 1-methoxydec-4-yl ester

Inchi: InChI=1S/C24H46O5/c1-6-7-8-10-14-22(15-13-18-27-5)29-24(26)17-12-9-11-16-23(25)2

InchiKey: ZOXWBTUPMWLKPV-UHFFFAOYSA-N

Formula: C24H46O5

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

Mol. weight [g/mol]: 414.62

Physical Properties

Property code	Value	Unit	Source
gf	-428.96	kJ/mol	Joback Method
hf	-1176.35	kJ/mol	Joback Method
hfus	54.11	kJ/mol	Joback Method
hvap	88.58	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	6.223		Crippen Method
mcvol	369.770	ml/mol	McGowan Method
pc	853.47	kPa	Joback Method
rinpol	2561.00		NIST Webbook
rinpol	2561.00		NIST Webbook
tb	922.20	K	Joback Method
tc	1130.13	K	Joback Method
tf	481.79	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.94	J/mol×K	922.20	Joback Method
cpg	1270.51	J/mol×K	956.86	Joback Method
cpg	1288.50	J/mol×K	991.51	Joback Method
cpg	1304.92	J/mol×K	1026.17	Joback Method
cpg	1319.79	J/mol×K	1060.82	Joback Method
cpg	1333.15	J/mol×K	1095.48	Joback Method
cpg	1345.01	J/mol×K	1130.13	Joback Method
dvisc	0.0005531	Pa×s	481.79	Joback Method

dvisc	0.0002092	Pa×s	555.19	Joback Method
dvisc	0.0000993	Pa×s	628.59	Joback Method
dvisc	0.0000551	Pa×s	702.00	Joback Method
dvisc	0.0000342	Pa×s	775.40	Joback Method
dvisc	0.0000230	Pa×s	848.80	Joback Method
dvisc	0.0000165	Pa×s	922.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406770&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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