Pimelic acid, 5-methoxy-3-methylpent-2-yl pentadecyl ester

Inchi: InChI=1S/C29H56O5/c1-5-6-7-8-9-10-11-12-13-14-15-16-20-24-33-28(30)21-18-17-19-2

InchiKey: BKTINWQNMXBDEN-UHFFFAOYSA-N

Formula: C29H56O5

SMILES: CCCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OC(C)C(C)CCOC

Mol. weight [g/mol]: 484.75

Physical Properties

Property code	Value	Unit	Source
gf	-384.42	kJ/mol	Joback Method
hf	-1274.27	kJ/mol	Joback Method
hfus	70.58	kJ/mol	Joback Method
hvap	100.09	kJ/mol	Joback Method
log10ws	-8.64		Crippen Method
logp	8.176		Crippen Method
mcvol	440.220	ml/mol	McGowan Method
pc	653.77	kPa	Joback Method
rinpol	3246.00		NIST Webbook
rinpol	3246.00		NIST Webbook
tb	1037.04	K	Joback Method
tc	1296.45	K	Joback Method
tf	553.14	K	Joback Method
vc	1.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1571.18	J/mol×K	1037.04	Joback Method
cpg	1593.30	J/mol×K	1080.28	Joback Method
cpg	1612.80	J/mol×K	1123.51	Joback Method
cpg	1629.75	J/mol×K	1166.75	Joback Method
cpg	1644.21	J/mol×K	1209.98	Joback Method
cpg	1656.27	J/mol×K	1253.22	Joback Method
cpg	1666.00	J/mol×K	1296.45	Joback Method
dvisc	0.0002316	Pa×s	553.14	Joback Method

dvisc	0.0000928	Pa×s	633.79	Joback Method
dvisc	0.0000457	Pa×s	714.44	Joback Method
dvisc	0.0000260	Pa×s	795.09	Joback Method
dvisc	0.0000164	Pa×s	875.74	Joback Method
dvisc	0.0000112	Pa×s	956.39	Joback Method
dvisc	0.0000081	Pa×s	1037.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406728&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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