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

Inchi: InChI=1S/C28H54O5/c1-5-6-7-8-9-10-11-12-13-14-15-19-23-32-27(29)20-17-16-18-21-2

InchiKey: LBYSNKYXGONGOP-UHFFFAOYSA-N

Formula: C28H54O5

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

Mol. weight [g/mol]: 470.73

Physical Properties

Property code	Value	Unit	Source
gf	-392.84	kJ/mol	Joback Method
hf	-1253.63	kJ/mol	Joback Method
hfus	67.99	kJ/mol	Joback Method
hvap	97.87	kJ/mol	Joback Method
log10ws	-8.23		Crippen Method
logp	7.785		Crippen Method
mcvol	426.130	ml/mol	McGowan Method
pc	687.09	kPa	Joback Method
rinpol	3147.00		NIST Webbook
rinpol	3147.00		NIST Webbook
tb	1014.16	K	Joback Method
tc	1260.67	K	Joback Method
tf	541.87	K	Joback Method
vc	1.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1506.49	J/mol×K	1014.16	Joback Method
cpg	1528.07	J/mol×K	1055.24	Joback Method
cpg	1547.31	J/mol×K	1096.33	Joback Method
cpg	1564.25	J/mol×K	1137.41	Joback Method
cpg	1578.95	J/mol×K	1178.50	Joback Method
cpg	1591.47	J/mol×K	1219.58	Joback Method
cpg	1601.87	J/mol×K	1260.67	Joback Method
dvisc	0.0002679	Pa×s	541.87	Joback Method

dvisc	0.0001080	Pa×s	620.59	Joback Method
dvisc	0.0000534	Pa×s	699.30	Joback Method
dvisc	0.0000305	Pa×s	778.01	Joback Method
dvisc	0.0000193	Pa×s	856.73	Joback Method
dvisc	0.0000132	Pa×s	935.44	Joback Method
dvisc	0.0000095	Pa×s	1014.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406727&Units=SI

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