Pimelic acid, 3-methyl-2-pentyl pentadecyl ester

Inchi: InChI=1S/C28H54O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-21-24-31-27(29)22-19-18-20-
InchiKey: DFQWJTQWWXSNMG-UHFFFAOYSA-N
Formula: C28H54O4
SMILES: CCCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OC(C)C(C)CC
Mol. weight [g/mol]: 454.73

Physical Properties

Property code	Value	Unit	Source
gf	-287.84	kJ/mol	Joback Method
hf	-1121.41	kJ/mol	Joback Method
hfus	66.80	kJ/mol	Joback Method
hvap	95.46	kJ/mol	Joback Method
log10ws	-9.14		Crippen Method
logp	8.549		Crippen Method
mcvol	420.260	ml/mol	McGowan Method
pc	693.25	kPa	Joback Method
rinpol	3062.00		NIST Webbook
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tb	991.74	K	Joback Method
tc	1227.53	K	Joback Method
tf	519.64	K	Joback Method
vc	1.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1475.15	J/mol×K	991.74	Joback Method
cpg	1497.37	J/mol×K	1031.04	Joback Method
cpg	1517.59	J/mol×K	1070.34	Joback Method
cpg	1535.87	J/mol×K	1109.64	Joback Method
cpg	1552.29	J/mol×K	1148.93	Joback Method
cpg	1566.92	J/mol×K	1188.23	Joback Method
cpg	1579.83	J/mol×K	1227.53	Joback Method
dvisc	0.0004088	Pa×s	519.64	Joback Method

dvisc	0.0001579	Pa×s	598.32	Joback Method
dvisc	0.0000761	Pa×s	677.01	Joback Method
dvisc	0.0000427	Pa×s	755.69	Joback Method
dvisc	0.0000267	Pa×s	834.37	Joback Method
dvisc	0.0000181	Pa×s	913.06	Joback Method
dvisc	0.0000131	Pa×s	991.74	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=U406605&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

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