Pimelic acid, dodecyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C27H52O4/c1-6-7-8-9-10-11-12-13-14-18-21-30-25(28)19-16-15-17-20-26(29)31-24-22-27(4,5)23-25(2)3

InchiKey: SAMJBNKITAAJFL-UHFFFAOYSA-N

Formula: C27H52O4

SMILES: CCCCCCCCCCCCOC(=O)CCCCCC(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	-290.98	kJ/mol	Joback Method
hf	-1104.24	kJ/mol	Joback Method
hfus	60.32	kJ/mol	Joback Method
hvap	92.32	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	8.017		Crippen Method
mcvol	406.170	ml/mol	McGowan Method
pc	734.03	kPa	Joback Method
rinpol	2078.00		NIST Webbook
rinpol	2078.00		NIST Webbook
tb	966.07	K	Joback Method
tc	1188.14	K	Joback Method
tf	525.79	K	Joback Method
vc	1.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1409.68	J/mol×K	966.07	Joback Method
cpg	1500.92	J/mol×K	1151.12	Joback Method
cpg	1485.63	J/mol×K	1114.11	Joback Method
cpg	1468.94	J/mol×K	1077.10	Joback Method
cpg	1450.77	J/mol×K	1040.09	Joback Method
cpg	1431.04	J/mol×K	1003.08	Joback Method
cpg	1514.88	J/mol×K	1188.14	Joback Method
dvisc	0.0000128	Pa×s	966.07	Joback Method

dvisc	0.0000178	Pa×s	892.69	Joback Method
dvisc	0.0000262	Pa×s	819.31	Joback Method
dvisc	0.0000418	Pa×s	745.93	Joback Method
dvisc	0.0000735	Pa×s	672.55	Joback Method
dvisc	0.0001487	Pa×s	599.17	Joback Method
dvisc	0.0003661	Pa×s	525.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406480&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