Pimelic acid, dodecyl octyl ester

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

InchiKey: SYNTYFNNBXKABI-UHFFFAOYSA-N

Formula: C27H52O4

SMILES: CCCCCCCCCCCCOC(=O)CCCCCC(=O)OCCCCCCCC

Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	-291.38	kJ/mol	Joback Method
hf	-1090.21	kJ/mol	Joback Method
hfus	71.26	kJ/mol	Joback Method
hvap	94.01	kJ/mol	Joback Method
log10ws	-8.85		Crippen Method
logp	8.305		Crippen Method
mcvol	406.170	ml/mol	McGowan Method
pc	723.40	kPa	Joback Method
rinpol	3057.00		NIST Webbook
tb	969.74	K	Joback Method
tc	1199.13	K	Joback Method
tf	538.37	K	Joback Method
vc	1.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1409.71	J/mol×K	969.74	Joback Method
cpg	1502.06	J/mol×K	1160.89	Joback Method
cpg	1487.05	J/mol×K	1122.66	Joback Method
cpg	1470.38	J/mol×K	1084.43	Joback Method
cpg	1451.97	J/mol×K	1046.20	Joback Method
cpg	1431.77	J/mol×K	1007.97	Joback Method
cpg	1515.46	J/mol×K	1199.13	Joback Method
dvisc	0.0000185	Pa×s	969.74	Joback Method
dvisc	0.0000248	Pa×s	897.85	Joback Method

dvisc	0.0000352	Pa×s	825.95	Joback Method
dvisc	0.0000532	Pa×s	754.06	Joback Method
dvisc	0.0000879	Pa×s	682.16	Joback Method
dvisc	0.0001634	Pa×s	610.26	Joback Method
dvisc	0.0003585	Pa×s	538.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393877&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