

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

Inchi:	InChI=1S/C27H52O4/c1-5-7-8-9-10-11-12-13-14-15-16-20-23-30-26(28)21-18-17-19-22-
InchiKey:	BSOUKGGXHMQRLLR-UHFFFAOYSA-N
Formula:	C27H52O4
SMILES:	CCCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)CC
Mol. weight [g/mol]:	440.70

Physical Properties

Property code	Value	Unit	Source
gf	-296.26	kJ/mol	Joback Method
hf	-1100.77	kJ/mol	Joback Method
hfus	64.21	kJ/mol	Joback Method
hvap	93.23	kJ/mol	Joback Method
log10ws	-8.72		Crippen Method
logp	8.159		Crippen Method
mvol	406.170	ml/mol	McGowan Method
pc	729.67	kPa	Joback Method
rinpol	2961.00		NIST Webbook
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tb	968.86	K	Joback Method
tc	1194.47	K	Joback Method
tf	508.37	K	Joback Method
vc	1.583	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.37	J/molxK	968.86	Joback Method
cpg	1500.78	J/molxK	1156.87	Joback Method
cpg	1486.11	J/molxK	1119.27	Joback Method
cpg	1469.79	J/molxK	1081.67	Joback Method
cpg	1451.77	J/molxK	1044.06	Joback Method
cpg	1431.98	J/molxK	1006.46	Joback Method
cpg	1513.86	J/molxK	1194.47	Joback Method
dvisc	0.0000153	Paxs	968.86	Joback Method

dvisc	0.0000212	Paxs	892.11	Joback Method
dvisc	0.0000312	Paxs	815.36	Joback Method
dvisc	0.0000498	Paxs	738.62	Joback Method
dvisc	0.0000886	Paxs	661.87	Joback Method
dvisc	0.0001832	Paxs	585.12	Joback Method
dvisc	0.0004716	Paxs	508.37	Joback Method

Sources

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=U406604&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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