

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

Inchi:	InChI=1S/C29H56O4/c1-6-7-8-9-10-11-12-13-14-15-16-20-23-32-27(30)21-18-17-19-22-
InchiKey:	RVBSJFGNAQHKFF-UHFFFAOYSA-N
Formula:	C29H56O4
SMILES:	CCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	468.75

Physical Properties

Property code	Value	Unit	Source
gf	-274.14	kJ/mol	Joback Method
hf	-1145.52	kJ/mol	Joback Method
hfus	65.50	kJ/mol	Joback Method
hvap	96.78	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	8.797		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	663.23	kPa	Joback Method
rinpol	2288.00		NIST Webbook
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tb	1011.83	K	Joback Method
tc	1253.72	K	Joback Method
tf	548.33	K	Joback Method
vc	1.690	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.55	J/molxK	1011.83	Joback Method
cpg	1634.74	J/molxK	1213.40	Joback Method
cpg	1619.12	J/molxK	1173.09	Joback Method
cpg	1601.90	J/molxK	1132.77	Joback Method
cpg	1582.97	J/molxK	1092.46	Joback Method
cpg	1562.22	J/molxK	1052.14	Joback Method
cpg	1648.87	J/molxK	1253.72	Joback Method
dvisc	0.0000092	Paxs	1011.83	Joback Method

dvisc	0.0000128	Paxs	934.58	Joback Method
dvisc	0.0000189	Paxs	857.33	Joback Method
dvisc	0.0000303	Paxs	780.08	Joback Method
dvisc	0.0000536	Paxs	702.83	Joback Method
dvisc	0.0001093	Paxs	625.58	Joback Method
dvisc	0.0002725	Paxs	548.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406482&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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