

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

Inchi:	InChI=1S/C26H50O4/c1-5-7-8-9-10-11-12-13-14-15-19-22-29-25(27)20-17-16-18-21-26(
InchiKey:	LBPVBCZSRJIJFC-UHFFFAOYSA-N
Formula:	C26H50O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)CC
Mol. weight [g/mol]:	426.67

Physical Properties

Property code	Value	Unit	Source
gf	-304.68	kJ/mol	Joback Method
hf	-1080.13	kJ/mol	Joback Method
hfus	61.62	kJ/mol	Joback Method
hvap	91.01	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.769		Crippen Method
mvol	392.080	ml/mol	McGowan Method
pc	769.04	kPa	Joback Method
rinpol	2860.00		NIST Webbook
rinpol	2860.00		NIST Webbook
tb	945.98	K	Joback Method
tc	1162.69	K	Joback Method
tf	497.10	K	Joback Method
vc	1.528	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.96	J/molxK	945.98	Joback Method
cpg	1367.00	J/molxK	982.10	Joback Method
cpg	1386.38	J/molxK	1018.22	Joback Method
cpg	1404.14	J/molxK	1054.33	Joback Method
cpg	1420.33	J/molxK	1090.45	Joback Method
cpg	1435.00	J/molxK	1126.57	Joback Method
cpg	1448.19	J/molxK	1162.69	Joback Method
dvisc	0.0005428	Paxs	497.10	Joback Method

dvisc	0.0002121	Paxs	571.91	Joback Method
dvisc	0.0001030	Paxs	646.73	Joback Method
dvisc	0.0000581	Paxs	721.54	Joback Method
dvisc	0.0000365	Paxs	796.35	Joback Method
dvisc	0.0000248	Paxs	871.17	Joback Method
dvisc	0.0000180	Paxs	945.98	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=U406603&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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