

Pimelic acid, 5-methoxy-3-methylpent-2-yl tridecyl ester

Inchi:	InChI=1S/C27H52O5/c1-5-6-7-8-9-10-11-12-13-14-18-22-31-26(28)19-16-15-17-20-27(2
InchiKey:	DWANHPDLJLMTEU-UHFFFAOYSA-N
Formula:	C27H52O5
SMILES:	CCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)CCOC
Mol. weight [g/mol]:	456.70

Physical Properties

Property code	Value	Unit	Source
gf	-401.26	kJ/mol	Joback Method
hf	-1232.99	kJ/mol	Joback Method
hfus	65.40	kJ/mol	Joback Method
hvap	95.64	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	7.395		Crippen Method
mcvol	412.040	ml/mol	McGowan Method
pc	723.02	kPa	Joback Method
rinsol	3047.00		NIST Webbook
tb	991.28	K	Joback Method
tc	1226.37	K	Joback Method
tf	530.60	K	Joback Method
vc	1.601	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1442.02	J/molxK	991.28	Joback Method
cpg	1463.10	J/molxK	1030.46	Joback Method
cpg	1482.05	J/molxK	1069.64	Joback Method
cpg	1498.93	J/molxK	1108.82	Joback Method
cpg	1513.79	J/molxK	1148.01	Joback Method
cpg	1526.67	J/molxK	1187.19	Joback Method
cpg	1537.61	J/molxK	1226.37	Joback Method
dvisc	0.0003092	Paxs	530.60	Joback Method
dvisc	0.0001254	Paxs	607.38	Joback Method

dvisc	0.0000623	Paxs	684.16	Joback Method
dvisc	0.0000356	Paxs	760.94	Joback Method
dvisc	0.0000226	Paxs	837.72	Joback Method
dvisc	0.0000155	Paxs	914.50	Joback Method
dvisc	0.0000112	Paxs	991.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406726&Units=SI

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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