

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

Inchi:	InChI=1S/C30H58O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-23-26-33-29(31)24-21-
InchiKey:	NLXSTOSRPKERDN-UHFFFAOYSA-N
Formula:	C30H58O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)CC
Mol. weight [g/mol]:	482.78

Physical Properties

Property code	Value	Unit	Source
gf	-271.00	kJ/mol	Joback Method
hf	-1162.69	kJ/mol	Joback Method
hfus	71.98	kJ/mol	Joback Method
hvap	99.91	kJ/mol	Joback Method
log10ws	-9.98		Crippen Method
logp	9.329		Crippen Method
mvol	448.440	ml/mol	McGowan Method
pc	628.14	kPa	Joback Method
rinpol	3262.00		NIST Webbook
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tb	1037.50	K	Joback Method
tc	1297.92	K	Joback Method
tf	542.18	K	Joback Method
vc	1.752	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1605.60	J/molxK	1037.50	Joback Method
cpg	1700.04	J/molxK	1254.52	Joback Method
cpg	1685.63	J/molxK	1211.11	Joback Method
cpg	1669.09	J/molxK	1167.71	Joback Method
cpg	1650.31	J/molxK	1124.31	Joback Method
cpg	1629.18	J/molxK	1080.90	Joback Method
cpg	1712.42	J/molxK	1297.92	Joback Method
dvisc	0.0000094	Paxs	1037.50	Joback Method

dvisc	0.0000131	Paxs	954.95	Joback Method
dvisc	0.0000194	Paxs	872.39	Joback Method
dvisc	0.0000312	Paxs	789.84	Joback Method
dvisc	0.0000558	Paxs	707.29	Joback Method
dvisc	0.0001167	Paxs	624.73	Joback Method
dvisc	0.0003054	Paxs	542.18	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=U406607&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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