

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

Inchi:	InChI=1S/C32H62O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-26-35-30(33)24-21-
InchiKey:	ZGVNBWLUBLWSBX-UHFFFAOYSA-N
Formula:	C32H62O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	510.83

Physical Properties

Property code	Value	Unit	Source
gf	-248.88	kJ/mol	Joback Method
hf	-1207.44	kJ/mol	Joback Method
hfus	73.27	kJ/mol	Joback Method
hvap	103.45	kJ/mol	Joback Method
log10ws	-10.46		Crippen Method
logp	9.967		Crippen Method
mvol	476.620	ml/mol	McGowan Method
pc	574.80	kPa	Joback Method
rinpol	2811.00		NIST Webbook
rinpol	2811.00		NIST Webbook
tb	1080.47	K	Joback Method
tc	1363.10	K	Joback Method
tf	582.14	K	Joback Method
vc	1.859	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1736.71	J/molxK	1080.47	Joback Method
cpg	1839.08	J/molxK	1315.99	Joback Method
cpg	1822.90	J/molxK	1268.89	Joback Method
cpg	1804.77	J/molxK	1221.78	Joback Method
cpg	1784.50	J/molxK	1174.68	Joback Method
cpg	1761.88	J/molxK	1127.57	Joback Method
cpg	1853.50	J/molxK	1363.10	Joback Method
dvisc	0.0000056	Paxs	1080.47	Joback Method

dvisc	0.0000078	Paxs	997.41	Joback Method
dvisc	0.0000115	Paxs	914.36	Joback Method
dvisc	0.0000185	Paxs	831.31	Joback Method
dvisc	0.0000330	Paxs	748.25	Joback Method
dvisc	0.0000681	Paxs	665.19	Joback Method
dvisc	0.0001728	Paxs	582.14	Joback Method

Sources

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=U406485&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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