

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

Inchi:	InChI=1S/C31H60O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-22-25-34-29(32)23-20-19-
InchiKey:	IGIISAASZGESIH-UHFFFAOYSA-N
Formula:	C31H60O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	496.81

Physical Properties

Property code	Value	Unit	Source
gf	-257.30	kJ/mol	Joback Method
hf	-1186.80	kJ/mol	Joback Method
hfus	70.68	kJ/mol	Joback Method
hvap	101.23	kJ/mol	Joback Method
log10ws	-10.04		Crippen Method
logp	9.577		Crippen Method
mvol	462.530	ml/mol	McGowan Method
pc	602.21	kPa	Joback Method
rinpol	2629.00		NIST Webbook
rinpol	2629.00		NIST Webbook
tb	1057.59	K	Joback Method
tc	1325.01	K	Joback Method
tf	570.87	K	Joback Method
vc	1.802	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1670.72	J/molxK	1057.59	Joback Method
cpg	1770.52	J/molxK	1280.44	Joback Method
cpg	1754.54	J/molxK	1235.87	Joback Method
cpg	1736.73	J/molxK	1191.30	Joback Method
cpg	1716.93	J/molxK	1146.73	Joback Method
cpg	1694.98	J/molxK	1102.16	Joback Method
cpg	1784.83	J/molxK	1325.01	Joback Method
dvisc	0.0000066	Paxs	1057.59	Joback Method

dvisc	0.0000092	Paxs	976.47	Joback Method
dvisc	0.0000136	Paxs	895.35	Joback Method
dvisc	0.0000218	Paxs	814.23	Joback Method
dvisc	0.0000389	Paxs	733.11	Joback Method
dvisc	0.0000799	Paxs	651.99	Joback Method
dvisc	0.0002015	Paxs	570.87	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=U406484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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