

9-Octadecenoic acid (Z)-, hexadecyl ester

Other names:	Oleic acid, hexadecyl ester Cetyl oleate Hexadecyl oleate Palmityl oleate Octadec-9-enoic acid hexadecyl ester, Z
Inchi:	InChI=1S/C34H66O2/c1-3-5-7-9-11-13-15-17-19-20-22-24-26-28-30-32-34(35)36-33-31-
InchiKey:	JYTMDBGMUIAIQH-ZPHPHTNESA-N
Formula:	C34H66O2
SMILES:	CCCCCCCC=CCCCCCCC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	506.89
CAS:	22393-86-8

Physical Properties

Property code	Value	Unit	Source
gf	81.70	kJ/mol	Joback Method
hf	-872.67	kJ/mol	Joback Method
hfus	86.81	kJ/mol	Joback Method
hvap	100.39	kJ/mol	Joback Method
log10ws	-12.77		Crippen Method
logp	12.048		Crippen Method
mcvol	493.060	ml/mol	McGowan Method
pc	520.31	kPa	Joback Method
rinpol	3520.42		NIST Webbook
rinpol	3520.42		NIST Webbook
tb	1057.77	K	Joback Method
tc	1345.09	K	Joback Method
tf	540.02	K	Joback Method
vc	1.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1790.65	J/molxK	1057.77	Joback Method
cpg	1821.08	J/molxK	1105.66	Joback Method

cpg	1849.08	J/molxK	1153.54	Joback Method
cpg	1874.90	J/molxK	1201.43	Joback Method
cpg	1898.79	J/molxK	1249.32	Joback Method
cpg	1920.99	J/molxK	1297.21	Joback Method
cpg	1941.76	J/molxK	1345.09	Joback Method
dvisc	0.0002583	Paxs	540.02	Joback Method
dvisc	0.0000966	Paxs	626.31	Joback Method
dvisc	0.0000458	Paxs	712.60	Joback Method
dvisc	0.0000255	Paxs	798.89	Joback Method
dvisc	0.0000159	Paxs	885.19	Joback Method
dvisc	0.0000108	Paxs	971.48	Joback Method
dvisc	0.0000078	Paxs	1057.77	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=C22393868&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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