

9-Hexadecenoic acid, octadecyl ester, (Z)-

Other names:	Hexadec-9-enoic acid octadecyl ester, Z
Inchi:	InChI=1S/C34H66O2/c1-3-5-7-9-11-13-15-17-18-19-21-23-25-27-29-31-33-36-34(35)32-
InchiKey:	OVIHKESDPWIFII-PEZBUJJGSA-N
Formula:	C34H66O2
SMILES:	CCCCCCC=CCCCCCCCC(=O)OCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	506.89
CAS:	22393-84-6

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	3528.96		NIST Webbook
rinpol	3528.96		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/mol×K	1057.77	Joback Method
cpg	1920.99	J/mol×K	1297.21	Joback Method
cpg	1898.79	J/mol×K	1249.32	Joback Method
cpg	1874.90	J/mol×K	1201.43	Joback Method
cpg	1849.08	J/mol×K	1153.54	Joback Method
cpg	1821.08	J/mol×K	1105.66	Joback Method

cpg	1941.76	J/mol×K	1345.09	Joback Method
dvisc	0.0000078	Pa×s	1057.77	Joback Method
dvisc	0.0000108	Pa×s	971.48	Joback Method
dvisc	0.0000159	Pa×s	885.19	Joback Method
dvisc	0.0000255	Pa×s	798.89	Joback Method
dvisc	0.0000458	Pa×s	712.60	Joback Method
dvisc	0.0000966	Pa×s	626.31	Joback Method
dvisc	0.0002583	Pa×s	540.02	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C22393846&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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