

Hexadecanoic acid hexadec-7-enyl ester, Z

Inchi:	InChI=1S/C32H62O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-34-32(33)30-28-26-
InchiKey:	PKBVRWLNWZPELG-HTXNQAPBSA-N
Formula:	C32H62O2
SMILES:	CCCCCCCC=CCCCCCCOC(=O)CCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	478.83

Physical Properties

Property code	Value	Unit	Source
gf	64.86	kJ/mol	Joback Method
hf	-831.39	kJ/mol	Joback Method
hfus	81.62	kJ/mol	Joback Method
hvap	95.94	kJ/mol	Joback Method
log10ws	-11.93		Crippen Method
logp	11.268		Crippen Method
mvol	464.880	ml/mol	McGowan Method
pc	569.06	kPa	Joback Method
rinpol	3328.91		NIST Webbook
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tb	1012.01	K	Joback Method
tc	1267.95	K	Joback Method
tf	517.48	K	Joback Method
vc	1.831	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1655.38	J/molxK	1012.01	Joback Method
cpg	1683.12	J/molxK	1054.67	Joback Method
cpg	1708.85	J/molxK	1097.32	Joback Method
cpg	1732.74	J/molxK	1139.98	Joback Method
cpg	1754.93	J/molxK	1182.64	Joback Method
cpg	1775.61	J/molxK	1225.29	Joback Method
cpg	1794.92	J/molxK	1267.95	Joback Method
dvisc	0.0003446	Paxs	517.48	Joback Method

dvisc	0.0001301	Paxs	599.90	Joback Method
dvisc	0.0000622	Paxs	682.32	Joback Method
dvisc	0.0000348	Paxs	764.74	Joback Method
dvisc	0.0000218	Paxs	847.17	Joback Method
dvisc	0.0000149	Paxs	929.59	Joback Method
dvisc	0.0000108	Paxs	1012.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R436772&Units=SI
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

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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