Tetradec-9-enoic acid octadecyl ester, Z

Inchi: InChI=1S/C32H62O2/c1-3-5-7-9-11-13-15-16-17-18-19-21-23-25-27-29-31-34-32(33)30-
InchiKey: XEYHWVLKUHJXGL-BENRWUELSA-N
Formula: C32H62O2
SMILES: CCCCC=CCCCCCCCC(=O)OCCCCCCCCCCCCCCCCCC
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
mcvol	464.880	ml/mol	McGowan Method
pc	569.06	kPa	Joback Method
rinpol	3340.55		NIST Webbook
rinpol	3340.55		NIST Webbook
tb	1012.01	K	Joback Method
tc	1267.95	K	Joback Method
tf	517.48	K	Joback Method
vc	1.831	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001301	Pa×s	599.90	Joback Method
dvisc	0.0000622	Pa×s	682.32	Joback Method
dvisc	0.0000348	Pa×s	764.74	Joback Method
dvisc	0.0000218	Pa×s	847.17	Joback Method
dvisc	0.0000149	Pa×s	929.59	Joback Method
dvisc	0.0000108	Pa×s	1012.01	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=R436861&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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