

Tetradec-9-enoic acid octadeca-9,12-dienyl ester, Z,Z,Z

Inchi:	InChI=1S/C32H58O2/c1-3-5-7-9-11-13-15-16-17-18-19-21-23-25-27-29-31-34-32(33)30-
InchiKey:	FVZCSSMNZNZORA-JUTWFEHOSA-N
Formula:	C32H58O2
SMILES:	CCCC=CCCCCCCC(=O)OCCCCCCCC=CCC=CCCCC
Mol. weight [g/mol]:	474.80

Physical Properties

Property code	Value	Unit	Source
gf	225.30	kJ/mol	Joback Method
hf	-596.95	kJ/mol	Joback Method
hfus	82.03	kJ/mol	Joback Method
hvap	95.86	kJ/mol	Joback Method
log10ws	-11.64		Crippen Method
logp	10.820		Crippen Method
mvol	456.280	ml/mol	McGowan Method
pc	598.38	kPa	Joback Method
rinpol	3308.64		NIST Webbook
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tb	1020.33	K	Joback Method
tc	1268.87	K	Joback Method
tf	507.32	K	Joback Method
vc	1.792	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1599.62	J/molxK	1020.33	Joback Method
cpg	1626.17	J/molxK	1061.75	Joback Method
cpg	1651.31	J/molxK	1103.18	Joback Method
cpg	1675.22	J/molxK	1144.60	Joback Method
cpg	1698.10	J/molxK	1186.02	Joback Method
cpg	1720.15	J/molxK	1227.44	Joback Method
cpg	1741.54	J/molxK	1268.87	Joback Method
dvisc	0.0003019	Paxs	507.32	Joback Method

dvisc	0.0001079	Paxs	592.82	Joback Method
dvisc	0.0000499	Paxs	678.32	Joback Method
dvisc	0.0000275	Paxs	763.83	Joback Method
dvisc	0.0000171	Paxs	849.33	Joback Method
dvisc	0.0000115	Paxs	934.83	Joback Method
dvisc	0.0000083	Paxs	1020.33	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=R437062&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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