

Octadeca-9,12-dienoic acid tetradecyl ester, Z

Inchi:	InChI=1S/C32H60O2/c1-3-5-7-9-11-13-15-17-18-19-20-22-24-26-28-30-32(33)34-31-29-
InchiKey:	KXYOLBNLWITKZ-BCTRXSSUSA-N
Formula:	C32H60O2
SMILES:	CCCCC=CCC=CCCCCCCCC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	476.82

Physical Properties

Property code	Value	Unit	Source
gf	145.08	kJ/mol	Joback Method
hf	-714.17	kJ/mol	Joback Method
hfus	81.83	kJ/mol	Joback Method
hvap	95.90	kJ/mol	Joback Method
log10ws	-11.79		Crippen Method
logp	11.044		Crippen Method
mcvol	460.580	ml/mol	McGowan Method
pc	583.44	kPa	Joback Method
rinpola	3315.74		NIST Webbook
tb	1016.17	K	Joback Method
tc	1268.18	K	Joback Method
tf	512.40	K	Joback Method
vc	1.812	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1627.52	J/molxK	1016.17	Joback Method
cpg	1654.62	J/molxK	1058.17	Joback Method
cpg	1680.02	J/molxK	1100.17	Joback Method
cpg	1703.89	J/molxK	1142.18	Joback Method
cpg	1726.40	J/molxK	1184.18	Joback Method
cpg	1747.75	J/molxK	1226.18	Joback Method
cpg	1768.11	J/molxK	1268.18	Joback Method
dvisc	0.0003224	Paxs	512.40	Joback Method
dvisc	0.0001185	Paxs	596.36	Joback Method

dvisc	0.0000557	Paxs	680.32	Joback Method
dvisc	0.0000309	Paxs	764.29	Joback Method
dvisc	0.0000193	Paxs	848.25	Joback Method
dvisc	0.0000131	Paxs	932.21	Joback Method
dvisc	0.0000095	Paxs	1016.17	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=R436534&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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