Hexadec-9-enoic acid hexadec-7-enyl ester, Z,Z

Inchi: InChI=1S/C32H60O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-34-32(33)30-28-26-

InchiKey: PFLNGJIHDARZBJ-JWCBKIGOSA-N

Formula: C32H60O2

SMILES: CCCCCCC=CCCCCCCCC(=O)OCCCCCCC=CCCCCCCCC

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
rinpol	3310.31		NIST Webbook
rinpol	3310.31		NIST Webbook
tb	1016.17	K	Joback Method
tc	1268.18	K	Joback Method
tf	512.40	K	Joback Method
vc	1.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1627.52	J/mol×K	1016.17	Joback Method
cpg	1654.62	J/mol×K	1058.17	Joback Method
cpg	1680.02	J/mol×K	1100.17	Joback Method
cpg	1703.89	J/mol×K	1142.18	Joback Method
cpg	1726.40	J/mol×K	1184.18	Joback Method
cpg	1747.75	J/mol×K	1226.18	Joback Method
cpg	1768.11	J/mol×K	1268.18	Joback Method
dvisc	0.0003224	Pa×s	512.40	Joback Method

dvisc	0.0001185	Pa×s	596.36	Joback Method
dvisc	0.0000557	Pa×s	680.32	Joback Method
dvisc	0.0000309	Pa×s	764.29	Joback Method
dvisc	0.0000193	Pa×s	848.25	Joback Method
dvisc	0.0000131	Pa×s	932.21	Joback Method
dvisc	0.0000095	Pa×s	1016.17	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=R436787&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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