Hexadec-9-enoic acid octadec-9-enyl ester, Z,Z

Other names: Hexadec-9-enoic acid octadec-9-enyl ester, Z,Z
Inchi: InChI=1S/C34H64O2/c1-3-5-7-9-11-13-15-17-18-19-21-23-25-27-29-31-33-36-34(35)32-
InchiKey: AJQOBPHRBMLQRX-LJSPAGPLSA-N
Formula: C34H64O2
SMILES: CCCCCC/C=C\CCCCCCCC(=O)OCCCCCCCC/C=C\CCCCCCC
Mol. weight [g/mol]: 504.88

Physical Properties

Property code	Value	Unit	Source
af	1.3112		Cheméo Relay (1.0)
gf	161.92	kJ/mol	Joback Method
hf	-934.16	kJ/mol	Cheméo Relay (1.0)
hfus	87.01	kJ/mol	Joback Method
hvap	156.74	kJ/mol	Cheméo Relay (1.0)
ie	8.82	eV	Cheméo Relay (1.0)
log10ws	-9.92		Cheméo Relay (1.0)
logp	11.824		Crippen Method
mcvol	488.760	ml/mol	McGowan Method
pc	532.87	kPa	Joback Method
rinpol	3503.04		NIST Webbook
rinpol	3503.04		NIST Webbook
tb	680.11	K	Cheméo Relay (1.0)
tc	878.08	K	Cheméo Relay (1.0)
tf	272.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1762.72	J/mol×K	1061.93	Joback Method
cpg	1792.61	J/mol×K	1108.85	Joback Method
cpg	1820.51	J/mol×K	1155.78	Joback Method
cpg	1846.68	J/mol×K	1202.70	Joback Method
cpg	1871.38	J/mol×K	1249.63	Joback Method
cpg	1894.89	J/mol×K	1296.55	Joback Method

cpg	1917.46	J/mol×K	1343.48	Joback Method
dvisc	0.0002416	Pa×s	534.94	Joback Method
dvisc	0.0000880	Pa×s	622.77	Joback Method
dvisc	0.0000411	Pa×s	710.60	Joback Method
dvisc	0.0000227	Pa×s	798.44	Joback Method
dvisc	0.0000141	Pa×s	886.27	Joback Method
dvisc	0.0000096	Pa×s	974.10	Joback Method
dvisc	0.0000069	Pa×s	1061.93	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22393982&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
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
ie: Ionization energy
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