Octadeca-9,12-dienoic acid hexadec-7-enyl ester, Z,Z,Z

Inchi: InChI=1S/C34H62O2/c1-3-5-7-9-11-13-15-17-19-20-22-24-26-28-30-32-34(35)36-33-31-
InchiKey: JUMWUQSFVUOQAA-RWYWNMNOSA-N
Formula: C34H62O2
SMILES: CCCCCC=CCC=CCCCCCCCC(=O)OCCCCCCC=CCCCCCCCC
Mol. weight [g/mol]: 502.85

Physical Properties

Property code	Value	Unit	Source
gf	242.14	kJ/mol	Joback Method
hf	-638.23	kJ/mol	Joback Method
hfus	87.21	kJ/mol	Joback Method
hvap	100.31	kJ/mol	Joback Method
log10ws	-12.48		Crippen Method
logp	11.600		Crippen Method
mcvol	484.460	ml/mol	McGowan Method
pc	545.90	kPa	Joback Method
rinpol	3497.40		NIST Webbook
tb	1066.09	K	Joback Method
tc	1342.37	K	Joback Method
tf	529.86	K	Joback Method
vc	1.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1734.78	J/mol×K	1066.09	Joback Method
cpg	1764.23	J/mol×K	1112.14	Joback Method
cpg	1792.10	J/mol×K	1158.18	Joback Method
cpg	1818.66	J/mol×K	1204.23	Joback Method
cpg	1844.18	J/mol×K	1250.28	Joback Method
cpg	1868.95	J/mol×K	1296.32	Joback Method
cpg	1893.25	J/mol×K	1342.37	Joback Method
dvisc	0.0002262	Pa×s	529.86	Joback Method
dvisc	0.0000801	Pa×s	619.23	Joback Method

dvisc	0.0000369	Pa×s	708.60	Joback Method
dvisc	0.0000202	Pa×s	797.98	Joback Method
dvisc	0.0000125	Pa×s	887.35	Joback Method
dvisc	0.0000084	Pa×s	976.72	Joback Method
dvisc	0.0000061	Pa×s	1066.09	Joback Method

Sources

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

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=R436816&Units=SI

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