Docosanoic acid hexadec-7-enyl ester, Z

Inchi: InChI=1S/C38H74O2/c1-3-5-7-9-11-13-15-17-19-20-21-22-23-24-26-28-30-32-34-36-38(
InchiKey: WWMRJCLIXZGJRE-XIEYBQDHSA-N
Formula: C38H74O2
SMILES: CCCCCCCCC=CCCCCCCOC(=O)CCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 562.99

Physical Properties

Property code	Value	Unit	Source
gf	115.38	kJ/mol	Joback Method
hf	-955.23	kJ/mol	Joback Method
hfus	97.17	kJ/mol	Joback Method
hvap	109.30	kJ/mol	Joback Method
log10ws	-14.45		Crippen Method
logp	13.609		Crippen Method
mcvol	549.420	ml/mol	McGowan Method
pc	439.87	kPa	Joback Method
rinpol	3931.84		NIST Webbook
tb	1149.29	K	Joback Method
tc	1523.64	K	Joback Method
tf	585.10	K	Joback Method
vc	2.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2064.62	J/mol×K	1149.29	Joback Method
cpg	2223.22	J/mol×K	1461.25	Joback Method
cpg	2196.10	J/mol×K	1398.86	Joback Method
cpg	2167.30	J/mol×K	1336.46	Joback Method
cpg	2136.19	J/mol×K	1274.07	Joback Method
cpg	2102.17	J/mol×K	1211.68	Joback Method
cpg	2249.29	J/mol×K	1523.64	Joback Method
dvisc	0.0000041	Pa×s	1149.29	Joback Method
dvisc	0.0000057	Pa×s	1055.26	Joback Method

dvisc	0.0000084	Pa×s	961.23	Joback Method
dvisc	0.0000135	Pa×s	867.19	Joback Method
dvisc	0.0000245	Pa×s	773.16	Joback Method
dvisc	0.0000522	Pa×s	679.13	Joback Method
dvisc	0.0001421	Pa×s	585.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R436856&Units=SI
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

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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