Hexadec-9-enoic acid docosyl ester, Z

Inchi: InChI=1S/C38H74O2/c1-3-5-7-9-11-13-15-17-18-19-20-21-22-23-25-27-29-31-33-35-37-
InchiKey: LKEQUAKZEFUZBG-PEZBUJJGSA-N
Formula: C38H74O2
SMILES: CCCCCCC=CCCCCCCCC(=O)OCCCCCCCCCCCCCCCCCCCCCC
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	3932.05		NIST Webbook
rinpol	3932.05		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	2102.17	J/mol×K	1211.68	Joback Method
cpg	2136.19	J/mol×K	1274.07	Joback Method
cpg	2167.30	J/mol×K	1336.46	Joback Method
cpg	2196.10	J/mol×K	1398.86	Joback Method
cpg	2223.22	J/mol×K	1461.25	Joback Method
cpg	2249.29	J/mol×K	1523.64	Joback Method
dvisc	0.0001421	Pa×s	585.10	Joback Method

dvisc	0.0000522	Pa×s	679.13	Joback Method
dvisc	0.0000245	Pa×s	773.16	Joback Method
dvisc	0.0000135	Pa×s	867.19	Joback Method
dvisc	0.0000084	Pa×s	961.23	Joback Method
dvisc	0.0000057	Pa×s	1055.26	Joback Method
dvisc	0.0000041	Pa×s	1149.29	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=R437344&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