Octadeca-9,12-dienoic acid docosyl ester, Z

Inchi: InChI=1S/C40H76O2/c1-3-5-7-9-11-13-15-17-19-20-21-22-23-25-27-29-31-33-35-37-39-
InchiKey: WBQCFLFBQKAZCD-IZZOXVKHSA-N
Formula: C40H76O2
SMILES: CCCCCC=CCC=CCCCCCCCC(=O)OCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 589.03

Physical Properties

Property code	Value	Unit	Source
gf	212.44	kJ/mol	Joback Method
hf	-879.29	kJ/mol	Joback Method
hfus	102.55	kJ/mol	Joback Method
hvap	113.71	kJ/mol	Joback Method
log10ws	-15.14		Crippen Method
logp	14.165		Crippen Method
mcvol	573.300	ml/mol	McGowan Method
pc	415.14	kPa	Joback Method
rinpol	4120.82		NIST Webbook
rinpol	4120.82		NIST Webbook
tb	1199.21	K	Joback Method
tc	1618.93	K	Joback Method
tf	602.56	K	Joback Method
vc	2.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2176.62	J/mol×K	1199.21	Joback Method
cpg	2219.48	J/mol×K	1269.16	Joback Method
cpg	2259.38	J/mol×K	1339.12	Joback Method
cpg	2297.34	J/mol×K	1409.07	Joback Method
cpg	2334.37	J/mol×K	1479.03	Joback Method
cpg	2371.50	J/mol×K	1548.98	Joback Method
cpg	2409.74	J/mol×K	1618.93	Joback Method
dvisc	0.0000976	Pa×s	602.56	Joback Method

dvisc	0.0000347	Pa×s	702.00	Joback Method
dvisc	0.0000160	Pa×s	801.44	Joback Method
dvisc	0.0000087	Pa×s	900.88	Joback Method
dvisc	0.0000054	Pa×s	1000.33	Joback Method
dvisc	0.0000036	Pa×s	1099.77	Joback Method
dvisc	0.0000026	Pa×s	1199.21	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=R437364&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