Octadeca-9,12,15-trienoic acid docosyl ester, Z,Z,Z

Inchi: InChI=1S/C40H74O2/c1-3-5-7-9-11-13-15-17-19-20-21-22-23-25-27-29-31-33-35-37-39-
InchiKey: FTWQNDJWUSTNNM-YABKDYGWSA-N
Formula: C40H74O2
SMILES: CCC=CCC=CCC=CCCCCCCCC(=O)OCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 587.01

Physical Properties

Property code	Value	Unit	Source
gf	292.66	kJ/mol	Joback Method
hf	-762.07	kJ/mol	Joback Method
hfus	102.75	kJ/mol	Joback Method
hvap	113.66	kJ/mol	Joback Method
log10ws	-14.99		Crippen Method
logp	13.941		Crippen Method
mcvol	569.000	ml/mol	McGowan Method
pc	424.07	kPa	Joback Method
rinpol	4129.59		NIST Webbook
rinpol	4129.59		NIST Webbook
tb	1203.37	K	Joback Method
tc	1610.47	K	Joback Method
tf	597.48	K	Joback Method
vc	2.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2150.40	J/mol×K	1203.37	Joback Method
cpg	2193.88	J/mol×K	1271.22	Joback Method
cpg	2235.50	J/mol×K	1339.07	Joback Method
cpg	2276.27	J/mol×K	1406.92	Joback Method
cpg	2317.22	J/mol×K	1474.77	Joback Method
cpg	2359.35	J/mol×K	1542.62	Joback Method
cpg	2403.69	J/mol×K	1610.47	Joback Method
dvisc	0.0000913	Pa×s	597.48	Joback Method

dvisc	0.0000317	Pa×s	698.46	Joback Method
dvisc	0.0000144	Pa×s	799.44	Joback Method
dvisc	0.0000078	Pa×s	900.42	Joback Method
dvisc	0.0000048	Pa×s	1001.41	Joback Method
dvisc	0.0000032	Pa×s	1102.39	Joback Method
dvisc	0.0000023	Pa×s	1203.37	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=R437379&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

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