Octadec-9-enoic acid docosyl ester, Z

Inchi: InChI=1S/C40H78O2/c1-3-5-7-9-11-13-15-17-19-20-21-22-23-25-27-29-31-33-35-37-39-
InchiKey: QKPJNZCOIFUYNE-MOHJPFBDSA-N
Formula: C40H78O2
SMILES: CCCCCCCCC=CCCCCCCCC(=O)OCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 591.05

Physical Properties

Property code	Value	Unit	Source
gf	132.22	kJ/mol	Joback Method
hf	-996.51	kJ/mol	Joback Method
hfus	102.34	kJ/mol	Joback Method
hvap	113.75	kJ/mol	Joback Method
log10ws	-15.28		Crippen Method
logp	14.389		Crippen Method
mcvol	577.600	ml/mol	McGowan Method
pc	406.48	kPa	Joback Method
rinpol	4124.07		NIST Webbook
rinpol	4124.07		NIST Webbook
tb	1195.05	K	Joback Method
tc	1628.18	K	Joback Method
tf	607.64	K	Joback Method
vc	2.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2203.01	J/mol×K	1195.05	Joback Method
cpg	2382.65	J/mol×K	1555.99	Joback Method
cpg	2351.05	J/mol×K	1483.81	Joback Method
cpg	2318.30	J/mol×K	1411.62	Joback Method
cpg	2283.38	J/mol×K	1339.43	Joback Method
cpg	2245.29	J/mol×K	1267.24	Joback Method
cpg	2414.11	J/mol×K	1628.18	Joback Method
dvisc	0.0000029	Pa×s	1195.05	Joback Method

dvisc	0.0000041	Pa×s	1097.15	Joback Method
dvisc	0.0000060	Pa×s	999.25	Joback Method
dvisc	0.0000098	Pa×s	901.35	Joback Method
dvisc	0.0000177	Pa×s	803.44	Joback Method
dvisc	0.0000381	Pa×s	705.54	Joback Method
dvisc	0.0001045	Pa×s	607.64	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=R437359&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