(Z)-(Z)-Docos-13-en-1-yl icos-11-enoate

Inchi: InChI=1S/C42H80O2/c1-3-5-7-9-11-13-15-17-19-21-22-23-25-27-29-31-33-35-37-39-41-
InchiKey: DKBUFWAUOWRWQE-CLFAGFIQSA-N
Formula: C42H80O2
SMILES: CCCCCCCCC=CCCCCCCCCCCCCCOC(=O)CCCCCCCCCC=CCCCCCCCC
Mol. weight [g/mol]: 617.08
CAS: 93036-93-2

Physical Properties

Property code	Value	Unit	Source
gf	229.28	kJ/mol	Joback Method
hf	-920.57	kJ/mol	Joback Method
hfus	107.73	kJ/mol	Joback Method
hvap	118.16	kJ/mol	Joback Method
log10ws	-15.97		Crippen Method
logp	14.945		Crippen Method
mcvol	601.480	ml/mol	McGowan Method
pc	384.47	kPa	Joback Method
rinpol	5018.30		NIST Webbook
rinpol	5018.30		NIST Webbook
tb	1244.97	K	Joback Method
tc	1732.83	K	Joback Method
tf	625.10	K	Joback Method
vc	2.372	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2317.06	J/mol×K	1244.97	Joback Method
cpg	2550.65	J/mol×K	1651.52	Joback Method
cpg	2503.35	J/mol×K	1570.21	Joback Method
cpg	2458.02	J/mol×K	1488.90	Joback Method
cpg	2412.98	J/mol×K	1407.59	Joback Method
cpg	2366.55	J/mol×K	1326.28	Joback Method
cpg	2601.58	J/mol×K	1732.83	Joback Method

dvisc	0.0000018	Pa×s	1244.97	Joback Method
dvisc	0.0000026	Pa×s	1141.66	Joback Method
dvisc	0.0000039	Pa×s	1038.35	Joback Method
dvisc	0.0000063	Pa×s	935.04	Joback Method
dvisc	0.0000115	Pa×s	831.72	Joback Method
dvisc	0.0000252	Pa×s	728.41	Joback Method
dvisc	0.0000714	Pa×s	625.10	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=C93036932&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