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

Inchi: InChI=1S/C30H56O2/c1-3-5-7-9-11-13-15-16-17-18-19-20-22-24-26-28-30(31)32-29-27-
InchiKey: YEVRRNZSZWIYCX-BIXSNLIQSA-N
Formula: C30H56O2
SMILES: CCCCCC=CCC=CCCCCCCCC(=O)OCCCCCCCCCCCC
Mol. weight [g/mol]: 448.76

Physical Properties

Property code	Value	Unit	Source
gf	128.24	kJ/mol	Joback Method
hf	-672.89	kJ/mol	Joback Method
hfus	76.65	kJ/mol	Joback Method
hvap	91.45	kJ/mol	Joback Method
log10ws	-10.95		Crippen Method
logp	10.264		Crippen Method
mcvol	432.400	ml/mol	McGowan Method
pc	641.57	kPa	Joback Method
rinpol	3116.66		NIST Webbook
rinpol	3116.66		NIST Webbook
tb	970.41	K	Joback Method
tc	1199.11	K	Joback Method
tf	489.86	K	Joback Method
vc	1.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1493.99	J/mol×K	970.41	Joback Method
cpg	1518.84	J/mol×K	1008.53	Joback Method
cpg	1542.22	J/mol×K	1046.64	Joback Method
cpg	1564.25	J/mol×K	1084.76	Joback Method
cpg	1585.06	J/mol×K	1122.88	Joback Method
cpg	1604.77	J/mol×K	1161.00	Joback Method
cpg	1623.51	J/mol×K	1199.11	Joback Method
dvisc	0.0004267	Pa×s	489.86	Joback Method

dvisc	0.0001583	Pa×s	569.95	Joback Method
dvisc	0.0000750	Pa×s	650.04	Joback Method
dvisc	0.0000419	Pa×s	730.13	Joback Method
dvisc	0.0000262	Pa×s	810.23	Joback Method
dvisc	0.0000179	Pa×s	890.32	Joback Method
dvisc	0.0000130	Pa×s	970.41	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=R436485&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