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

Inchi: InChI=1S/C30H54O2/c1-3-5-7-9-11-13-15-16-17-18-19-20-22-24-26-28-30(31)32-29-27-

InchiKey: OJUWCMVWZKGKMF-YYPVPKODSA-N

Formula: C30H54O2

SMILES: CCC=CCC=CCC=CCCCCCCCC(=O)OCCCCCCCCCCCCC

Mol. weight [g/mol]: 446.75

Physical Properties

Property code	Value	Unit	Source
gf	208.46	kJ/mol	Joback Method
hf	-555.67	kJ/mol	Joback Method
hfus	76.85	kJ/mol	Joback Method
hvap	91.40	kJ/mol	Joback Method
log10ws	-10.80		Crippen Method
logp	10.040		Crippen Method
mcvol	428.100	ml/mol	McGowan Method
pc	658.81	kPa	Joback Method
rinpol	3123.04		NIST Webbook
rinpol	3123.04		NIST Webbook
tb	974.57	K	Joback Method
tc	1201.38	K	Joback Method
tf	484.78	K	Joback Method
vc	1.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1466.37	J/mol×K	974.57	Joback Method
cpg	1576.37	J/mol×K	1163.58	Joback Method
cpg	1556.35	J/mol×K	1125.77	Joback Method
cpg	1535.47	J/mol×K	1087.97	Joback Method
cpg	1513.61	J/mol×K	1050.17	Joback Method
cpg	1490.62	J/mol×K	1012.37	Joback Method
cpg	1595.68	J/mol×K	1201.38	Joback Method
dvisc	0.0000114	Pa×s	974.57	Joback Method

dvisc	0.0000157	Pa×s	892.94	Joback Method
dvisc	0.0000231	Pa×s	811.31	Joback Method
dvisc	0.0000371	Pa×s	729.67	Joback Method
dvisc	0.0000671	Pa×s	648.04	Joback Method
dvisc	0.0001440	Pa×s	566.41	Joback Method
dvisc	0.0003996	Pa×s	484.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R436490&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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