Octadec-9-enoic acid dodecyl ester, Z

Inchi: InChI=1S/C30H58O2/c1-3-5-7-9-11-13-15-16-17-18-19-20-22-24-26-28-30(31)32-29-27-
InchiKey: OXPCWUWUWIWSGI-MSUUIHNZSA-N
Formula: C30H58O2
SMILES: CCCCCCCCC=CCCCCCCCC(=O)OCCCCCCCCCCCC
Mol. weight [g/mol]: 450.78

Physical Properties

Property code	Value	Unit	Source
gf	48.02	kJ/mol	Joback Method
hf	-790.11	kJ/mol	Joback Method
hfus	76.45	kJ/mol	Joback Method
hvap	91.49	kJ/mol	Joback Method
log10ws	-11.10		Crippen Method
logp	10.488		Crippen Method
mcvol	436.700	ml/mol	McGowan Method
pc	625.00	kPa	Joback Method
rinpol	3122.55		NIST Webbook
rinpol	3122.55		NIST Webbook
tb	966.25	K	Joback Method
tc	1197.27	K	Joback Method
tf	494.94	K	Joback Method
vc	1.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1521.52	J/mol×K	966.25	Joback Method
cpg	1633.42	J/mol×K	1158.77	Joback Method
cpg	1613.97	J/mol×K	1120.26	Joback Method
cpg	1593.16	J/mol×K	1081.76	Joback Method
cpg	1570.90	J/mol×K	1043.26	Joback Method
cpg	1547.05	J/mol×K	1004.75	Joback Method
cpg	1651.64	J/mol×K	1197.27	Joback Method
dvisc	0.0000148	Pa×s	966.25	Joback Method

dvisc	0.0000203	Pa×s	887.70	Joback Method
dvisc	0.0000297	Pa×s	809.15	Joback Method
dvisc	0.0000472	Pa×s	730.60	Joback Method
dvisc	0.0000838	Pa×s	652.04	Joback Method
dvisc	0.0001740	Pa×s	573.49	Joback Method
dvisc	0.0004559	Pa×s	494.94	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=R436470&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