9-Hexadecenoic acid, tetradecyl ester, (Z)-

Other names: Hexadec-9-enoic acid tetradecyl ester, Z
Inchi: InChI=1S/C30H58O2/c1-3-5-7-9-11-13-15-17-18-20-22-24-26-28-30(31)32-29-27-25-23-
InchiKey: RSXGJFMEKMHQAN-SQFISAMPSA-N
Formula: C30H58O2
SMILES: CCCCCCC=CCCCCCCCC(=O)OCCCCCCCCCCCCCC
Mol. weight [g/mol]: 450.78
CAS: 22393-82-4

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	3129.40		NIST Webbook
rinpol	3129.40		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	1547.05	J/mol×K	1004.75	Joback Method
cpg	1570.90	J/mol×K	1043.26	Joback Method
cpg	1593.16	J/mol×K	1081.76	Joback Method
cpg	1613.97	J/mol×K	1120.26	Joback Method
cpg	1633.42	J/mol×K	1158.77	Joback Method

cpg	1651.64	J/mol×K	1197.27	Joback Method
dvisc	0.0004559	Pa×s	494.94	Joback Method
dvisc	0.0001740	Pa×s	573.49	Joback Method
dvisc	0.0000838	Pa×s	652.04	Joback Method
dvisc	0.0000472	Pa×s	730.60	Joback Method
dvisc	0.0000297	Pa×s	809.15	Joback Method
dvisc	0.0000203	Pa×s	887.70	Joback Method
dvisc	0.0000148	Pa×s	966.25	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22393824&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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