

Tetradec-9-enoic acid hexadecyl ester, Z

Inchi:	InChI=1S/C30H58O2/c1-3-5-7-9-11-13-15-16-17-19-21-23-25-27-29-32-30(31)28-26-24-
InchiKey:	DYIOQMKBPSAFY-BENRWUELSA-N
Formula:	C30H58O2
SMILES:	CCCC=CCCCCCCC(=O)OCCCCCCCCCCCCCCCC
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
mvol	436.700	ml/mol	McGowan Method
pc	625.00	kPa	Joback Method
rinpol	3140.65		NIST Webbook
rinpol	3140.65		NIST Webbook
tb	966.25	K	Joback Method
tc	1197.27	K	Joback Method
tf	494.94	K	Joback Method
vc	1.720	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1521.52	J/molxK	966.25	Joback Method
cpg	1547.05	J/molxK	1004.75	Joback Method
cpg	1570.90	J/molxK	1043.26	Joback Method
cpg	1593.16	J/molxK	1081.76	Joback Method
cpg	1613.97	J/molxK	1120.26	Joback Method
cpg	1633.42	J/molxK	1158.77	Joback Method
cpg	1651.64	J/molxK	1197.27	Joback Method
dvisc	0.0004559	Paxs	494.94	Joback Method

dvisc	0.0001740	Paxs	573.49	Joback Method
dvisc	0.0000838	Paxs	652.04	Joback Method
dvisc	0.0000472	Paxs	730.60	Joback Method
dvisc	0.0000297	Paxs	809.15	Joback Method
dvisc	0.0000203	Paxs	887.70	Joback Method
dvisc	0.0000148	Paxs	966.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R436683&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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