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

Other names:	Hexadec-9-enoic acid icosyl ester, Z
Inchi:	InChI=1S/C36H70O2/c1-3-5-7-9-11-13-15-17-18-19-20-21-23-25-27-29-31-33-35-38-36(
InchiKey:	FIETWBRPSYJUOM-PEZBUJJGSA-N
Formula:	C36H70O2
SMILES:	CCCCCCC=CCCCCCCCC(=O)OCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	534.94
CAS:	22522-34-5

Physical Properties

Property code	Value	Unit	Source
gf	98.54	kJ/mol	Joback Method
hf	-913.95	kJ/mol	Joback Method
hfus	91.99	kJ/mol	Joback Method
hvap	104.84	kJ/mol	Joback Method
log10ws	-13.61		Crippen Method
logp	12.829		Crippen Method
mcvol	521.240	ml/mol	McGowan Method
pc	477.56	kPa	Joback Method
rinpol	3730.31		NIST Webbook
rinpol	3730.31		NIST Webbook
tb	1103.53	K	Joback Method
tc	1429.86	K	Joback Method
tf	562.56	K	Joback Method
vc	2.055	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1927.12	J/mol×K	1103.53	Joback Method
cpg	1960.79	J/mol×K	1157.92	Joback Method
cpg	1991.51	J/mol×K	1212.31	Joback Method
cpg	2019.68	J/mol×K	1266.69	Joback Method
cpg	2045.69	J/mol×K	1321.08	Joback Method
cpg	2069.92	J/mol×K	1375.47	Joback Method

cpg	2092.76	J/mol×K	1429.86	Joback Method
dvisc	0.0001922	Pa×s	562.56	Joback Method
dvisc	0.0000712	Pa×s	652.72	Joback Method
dvisc	0.0000336	Pa×s	742.88	Joback Method
dvisc	0.0000186	Pa×s	833.04	Joback Method
dvisc	0.0000116	Pa×s	923.21	Joback Method
dvisc	0.0000078	Pa×s	1013.37	Joback Method
dvisc	0.0000057	Pa×s	1103.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22522345&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

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