

Linoelaidic acid

Inchi:	InChI=1S/C18H32O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h6-7,9-10H,
InchiKey:	OYHQOLUKZRVURQ-AVQMFFATSA-N
Formula:	C18H32O2
SMILES:	CCCCC=CCC=CCCCCCCC(=O)O
Mol. weight [g/mol]:	280.45
CAS:	506-21-8

Physical Properties

Property code	Value	Unit	Source
gf	-4.62	kJ/mol	Joback Method
hf	-445.22	kJ/mol	Joback Method
hfl	-640.20	kJ/mol	NIST Webbook
hfus	48.47	kJ/mol	Joback Method
hvap	79.00	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.885		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
tb	765.61	K	Joback Method
tc	944.34	K	Joback Method
tf	393.21	K	Joback Method
vc	1.028	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.21	J/molxK	944.34	Joback Method
cpg	787.02	J/molxK	765.61	Joback Method
cpg	802.93	J/molxK	795.40	Joback Method
cpg	818.10	J/molxK	825.19	Joback Method
cpg	832.56	J/molxK	854.97	Joback Method
cpg	846.37	J/molxK	884.76	Joback Method
cpg	859.57	J/molxK	914.55	Joback Method
dvisc	0.0000180	Paxs	765.61	Joback Method

dvisc	0.0023129	Paxs	393.21	Joback Method
dvisc	0.0005934	Paxs	455.28	Joback Method
dvisc	0.0002110	Paxs	517.34	Joback Method
dvisc	0.0000937	Paxs	579.41	Joback Method
dvisc	0.0000486	Paxs	641.48	Joback Method
dvisc	0.0000284	Paxs	703.54	Joback Method
hfust	47.70	kJ/mol	303.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C506218&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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