

Linolene aldehyde

Inchi:	InChI=1S/C18H30O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h3-4,6-7,9-10,18
InchiKey:	TUCMDDWTBVMRTP-PDBXOOCHSA-N
Formula:	C18H30O
SMILES:	CCC=CCC=CCC=CCCCCCCCC=O
Mol. weight [g/mol]:	262.43

Physical Properties

Property code	Value	Unit	Source
gf	241.82	kJ/mol	Joback Method
hf	-148.77	kJ/mol	Joback Method
hfus	45.27	kJ/mol	Joback Method
hvap	62.26	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.775		Crippen Method
mcvol	253.150	ml/mol	McGowan Method
pc	1355.63	kPa	Joback Method
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook
tb	672.38	K	Joback Method
tc	851.25	K	Joback Method
tf	319.38	K	Joback Method
vc	1.000	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.79	J/mol×K	672.38	Joback Method
cpg	772.11	J/mol×K	821.43	Joback Method
cpg	757.72	J/mol×K	791.62	Joback Method
cpg	742.65	J/mol×K	761.81	Joback Method
cpg	726.84	J/mol×K	732.00	Joback Method
cpg	710.24	J/mol×K	702.19	Joback Method
cpg	785.87	J/mol×K	851.25	Joback Method
dvisc	0.0000876	Paxs	672.38	Joback Method

dvisc	0.0001186	Paxs	613.55	Joback Method
dvisc	0.0001713	Paxs	554.71	Joback Method
dvisc	0.0002699	Paxs	495.88	Joback Method
dvisc	0.0004808	Paxs	437.05	Joback Method
dvisc	0.0010250	Paxs	378.21	Joback Method
dvisc	0.0028878	Paxs	319.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R233815&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
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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