

Longifolenaldehyde

Other names:	Longifolenealdehyde
Inchi:	InChI=1S/C15H24O/c1-14(2)7-4-8-15(3)11-6-5-10(13(11)14)12(15)9-16/h9-13H,4-8H2,1
InchiKey:	PBMHTGOFWRRJFS-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CC1(C)CCCC2(C)C(C=O)C3CCC2C31
Mol. weight [g/mol]:	220.35
CAS:	19890-84-7

Physical Properties

Property code	Value	Unit	Source
gf	99.84	kJ/mol	Joback Method
hf	-262.97	kJ/mol	Joback Method
hfus	17.72	kJ/mol	Joback Method
hvap	52.56	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.674		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	1631.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1668.00		NIST Webbook
tb	606.49	K	Joback Method
tc	831.12	K	Joback Method
tf	382.67	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.11	J/molxK	606.49	Joback Method
cpg	575.51	J/molxK	643.93	Joback Method
cpg	596.54	J/molxK	681.37	Joback Method
cpg	616.51	J/molxK	718.81	Joback Method
cpg	635.69	J/molxK	756.25	Joback Method

cpg	654.37	J/mol×K	793.69	Joback Method
cpg	672.85	J/mol×K	831.12	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19890847&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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