4,8,12-Tetradecatrienal, 5,9,13-trimethyl-

Other names: Farnesyl acetaldehyde
Inchi: InChI=1S/C17H28O/c1-15(2)9-7-11-17(4)13-8-12-16(3)10-5-6-14-18/h9-10,13-14H,5-8,1
InchiKey: IDHMAJKSCCNULC-QKXOVSGLSA-N
Formula: C17H28O
SMILES: CC(C)=CCCC(C)=CCCC(C)=CCCC=O
Mol. weight [g/mol]: 248.40
CAS: 66408-55-7

Physical Properties

Property code	Value	Unit	Source
gf	207.75	kJ/mol	Joback Method
hf	-157.50	kJ/mol	Joback Method
hfus	38.75	kJ/mol	Joback Method
hvap	60.27	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.385		Crippen Method
mcvol	239.060	ml/mol	McGowan Method
pc	1473.62	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
tb	649.14	K	Joback Method
tc	836.08	K	Joback Method
tf	266.23	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.81	J/mol×K	649.14	Joback Method
cpg	654.49	J/mol×K	680.30	Joback Method
cpg	671.27	J/mol×K	711.45	Joback Method
cpg	687.20	J/mol×K	742.61	Joback Method
cpg	702.35	J/mol×K	773.77	Joback Method
cpg	716.78	J/mol×K	804.93	Joback Method

cpg	730.56	J/mol×K	836.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66408557&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
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