5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl-, (E,E)-

Other names: Farnesyl acetone
5,9,13-Pentadecatrien-2-one, 6,10,14-trimethhyl-, [E,E]
(E,E)-6,10,14-trimethylpentadeca-5,9,13-trien-2-one

Inchi: InChI=1S/C18H30O/c1-15(2)9-6-10-16(3)11-7-12-17(4)13-8-14-18(5)19/h9,11,13H,6-8,1

InchiKey: LTUMRKDLVGQMJU-IUBLYSDUSA-N

Formula: C18H30O

SMILES: CC(=O)CCC=C(C)CCC=C(C)CCC=C(C)C

Mol. weight [g/mol]: 262.43

CAS: 1117-52-8

Physical Properties

Property code	Value	Unit	Source
gf	186.77	kJ/mol	Joback Method
hf	-205.14	kJ/mol	Joback Method
hfus	40.65	kJ/mol	Joback Method
hvap	62.52	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.775		Crippen Method
mcvol	253.150	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	1895.00		NIST Webbook
rinpol	1914.00		NIST Webbook
rinpol	1881.00		NIST Webbook
rinpol	1886.00		NIST Webbook
rinpol	1893.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1921.00		NIST Webbook
rinpol	1892.00		NIST Webbook
rinpol	1919.00		NIST Webbook
rinpol	1933.00		NIST Webbook
rinpol	1911.00		NIST Webbook
rinpol	1911.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1911.00		NIST Webbook
rinpol	1922.40		NIST Webbook
rinpol	1919.00		NIST Webbook
rinpol	1918.00		NIST Webbook

rinpol	1895.00		NIST Webbook
rinpol	1913.00		NIST Webbook
rinpol	1919.00		NIST Webbook
rinpol	1919.00		NIST Webbook
rinpol	1914.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	1913.00		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	1881.00		NIST Webbook
rinpol	1916.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1919.00		NIST Webbook
rinpol	1919.80		NIST Webbook
rinpol	1918.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1892.00		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	1914.00		NIST Webbook
rinpol	1927.00		NIST Webbook
ripol	2363.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2386.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2386.00		NIST Webbook
ripol	2386.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2364.00		NIST Webbook
ripol	2375.00		NIST Webbook
ripol	2376.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2376.00		NIST Webbook
ripol	2363.00		NIST Webbook
ripol	2376.00		NIST Webbook
ripol	2376.00		NIST Webbook
tb	677.23	K	Joback Method

tc	866.12	K	Joback Method
tf	285.43	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.45	J/mol×K	677.23	Joback Method
cpg	710.76	J/mol×K	708.71	Joback Method
cpg	728.14	J/mol×K	740.19	Joback Method
cpg	744.65	J/mol×K	771.68	Joback Method
cpg	760.37	J/mol×K	803.16	Joback Method
cpg	775.34	J/mol×K	834.64	Joback Method
cpg	789.64	J/mol×K	866.12	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1117528&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

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume