2-Pentadecanone, 6,10,14-trimethyl-

Other names:	Hexahydrofarnesyl acetone
	6,10,14-Trimethyl-2-pentadecanone
	6,10,14-Trimethylpentadecan-2-one
	Perhydrofarnesyl acetone
Inchi:	InChI=1S/C18H36O/c1-15(2)9-6-10-16(3)11-7-12-17(4)13-8-14-18(5)19/h15-17H,6-14H2
InchiKey:	WHWDWIHXSPCOKZ-UHFFFAOYSA-N
Formula:	C18H36O
SMILES:	CC(=O)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]:	268.48
CAS:	502-69-2

Physical Properties

Property code	Value	Unit	Source
chl	-11602.00 ± 5.20	kJ/mol	NIST Webbook
chl	-11596.70	kJ/mol	NIST Webbook
gf	-35.56	kJ/mol	Joback Method
hf	-543.27	kJ/mol	Joback Method
hfl	-631.40 ± 9.20	kJ/mol	NIST Webbook
hfl	-626.10 ± 2.30	kJ/mol	NIST Webbook
hfus	33.41	kJ/mol	Joback Method
hvap	61.24	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	6.015		Crippen Method
mcvol	266.050	ml/mol	McGowan Method
pc	1223.41	kPa	Joback Method
rinpol	1843.00		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1845.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1798.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1845.00		NIST Webbook
rinpol	1848.00		NIST Webbook
rinpol	1848.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1801.00		NIST Webbook

rinpol	1830.00		NIST Webbook
rinpol	1801.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1846.70		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1798.00		NIST Webbook
rinpol	1848.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1846.70		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1864.00		NIST Webbook
ripol	2131.00		NIST Webbook
ripol	2114.00		NIST Webbook
ripol	2131.00		NIST Webbook
ripol	2125.00		NIST Webbook
ripol	2129.00		NIST Webbook
ripol	2131.00		NIST Webbook
ripol	2131.00		NIST Webbook
ripol	2110.00		NIST Webbook
ripol	2131.00		NIST Webbook
tb	663.79	K	Joback Method
tc	837.19	K	Joback Method
tf	297.55	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.01	J/mol×K	663.79	Joback Method
cpg	864.76	J/mol×K	837.19	Joback Method

cpg	849.23	J/mol×K	808.29	Joback Method
cpg	832.90	J/mol×K	779.39	Joback Method
cpg	815.74	J/mol×K	750.49	Joback Method
cpg	797.72	J/mol×K	721.59	Joback Method
cpg	778.82	J/mol×K	692.69	Joback Method
cpl	593.30	J/mol×K	293.85	NIST Webbook
dvisc	0.0020519	Pa×s	358.59	Joback Method
dvisc	0.0000989	Pa×s	663.79	Joback Method
dvisc	0.0001419	Pa×s	602.75	Joback Method
dvisc	0.0002208	Pa×s	541.71	Joback Method
dvisc	0.0003843	Pa×s	480.67	Joback Method
dvisc	0.0007862	Pa×s	419.63	Joback Method
dvisc	0.0079383	Pa×s	297.55	Joback Method
hvapt	56.00 ± 0.60	kJ/mol	451.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C502692&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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

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