Nootkatone

Other names:	2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, [4R-(4«alpha»,4a«alpha»,6«beta»)]-
	(4R,4aS,6R)-4,4a-Dimethyl-6-(prop-1-en-2-yl)-4,4a,5,6,7,8-hexahydronaphthalen-2(3H)-o
	4«beta»H,5«alpha»-Eremophila-1(10),11-dien-2-one
	4«beta»H,5«alpha»-Eremorphila-1(10)11-dien-2-one
	4,4a,5,6,7,8-Hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-2(3H)-naphthalenone, [4R-(4«alpha»,4a«alpha»,6«beta»)]-
	6-Isopropenyl-4,4a-dimethyl-4,4a,5,6,7,8-hexahydro-2(3H)-naphthalenone-, [4R-(4«alpha»,4a«alpha»,6«beta»)]-
	(+)-5,6-dimethyl-8-isopropenylbicyclo[4.4.0]dec-1-en-3-one
	2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)-
	(+)-Nootkatone
	Nootkanone
	Nootkatane
	[4R-(4«alpha»,4a«alpha»,6«beta»)]-4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylvin
Inchi:	InChI=1S/C15H22O/c1-10(2)12-5-6-13-8-14(16)7-11(3)15(13,4)9-12/h8,11-12H,1,5-7,9H
InchiKey:	WTOYNNBCKUYIKC-SLEUVZQESA-N
Formula:	C15H22O
SMILES:	C=C(C)C1CCC2=CC(=O)CC(C)C2(C)C1
Mol. weight [g/mol]:	218.33
CAS:	4674-50-4

Physical Properties

Property code	Value	Unit	Source
gf	112.35	kJ/mol	Joback Method
hf	-212.82	kJ/mol	Joback Method
hfus	15.00	kJ/mol	Joback Method
hvap	52.65	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1780.00		NIST Webbook
rinpol	1834.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1798.00		NIST Webbook
rinpol	1819.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1834.00		NIST Webbook
rinpol	1833.00		NIST Webbook

rinpol	1800.00	NIST Webbook
rinpol	1780.00	NIST Webbook
rinpol	1775.00	NIST Webbook
rinpol	1780.00	NIST Webbook
rinpol	1780.00	NIST Webbook
rinpol	1803.00	NIST Webbook
rinpol	1781.00	NIST Webbook
rinpol	1780.00	NIST Webbook
rinpol	1837.00	NIST Webbook
rinpol	1814.00	NIST Webbook
rinpol	1820.00	NIST Webbook
rinpol	1814.00	NIST Webbook
rinpol	1814.00	NIST Webbook
rinpol	1822.00	NIST Webbook
rinpol	1820.00	NIST Webbook
rinpol	1820.00	NIST Webbook
rinpol	1820.00	NIST Webbook
rinpol	1802.00	NIST Webbook
rinpol	1799.00	NIST Webbook
rinpol	1794.00	NIST Webbook
rinpol	1774.00	NIST Webbook
rinpol	1775.00	NIST Webbook
rinpol	1799.00	NIST Webbook
rinpol	1802.00	NIST Webbook
rinpol	1834.00	NIST Webbook
rinpol	1835.00	NIST Webbook
rinpol	1751.00	NIST Webbook
rinpol	1790.00	NIST Webbook
rinpol	1823.00	NIST Webbook
rinpol	1798.00	NIST Webbook
rinpol	1775.00	NIST Webbook
rinpol	1765.00	NIST Webbook
rinpol	1775.00	NIST Webbook
rinpol	1801.00	NIST Webbook
rinpol	1798.00	NIST Webbook
rinpol	1805.00	NIST Webbook
rinpol	1806.00	NIST Webbook
rinpol	1807.00	NIST Webbook
rinpol	1810.00	NIST Webbook
rinpol	1819.00	NIST Webbook
rinpol	1800.00	NIST Webbook
rinpol	1812.00	NIST Webbook
rinpol	1833.00	NIST Webbook
rinpol	1816.00	NIST Webbook

rinpol	1797.00		NIST Webbook
rinpol	1781.00		NIST Webbook
rinpol	1807.00		NIST Webbook
rinpol	1797.00		NIST Webbook
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rinpol	1807.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1794.00		NIST Webbook
rinpol	1834.00		NIST Webbook
rinpol	1798.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1780.00		NIST Webbook
ripol	2527.00		NIST Webbook
ripol	2506.00		NIST Webbook
ripol	2515.00		NIST Webbook
ripol	2525.00		NIST Webbook
ripol	2526.00		NIST Webbook
ripol	2532.00		NIST Webbook
ripol	2563.00		NIST Webbook
ripol	2563.00		NIST Webbook
ripol	2544.00		NIST Webbook
ripol	2504.00		NIST Webbook
ripol	2539.00		NIST Webbook
ripol	2554.00		NIST Webbook
ripol	2515.00		NIST Webbook
ripol	2515.00		NIST Webbook
ripol	2527.00		NIST Webbook
ripol	2563.00		NIST Webbook
ripol	2563.00		NIST Webbook
ripol	2522.00		NIST Webbook
tb	637.25	K	Joback Method
tc	875.13	K	Joback Method
tf	366.05	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.13	J/mol×K	637.25	Joback Method
cpg	562.46	J/mol×K	676.90	Joback Method

cpg	583.51	J/mol×K	716.54	Joback Method
cpg	603.42	J/mol×K	756.19	Joback Method
cpg	622.34	J/mol×K	795.83	Joback Method
cpg	640.42	J/mol×K	835.48	Joback Method
cpg	657.81	J/mol×K	875.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4674504&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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