2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methyle (4R-cis)-

Other names:	(4R,4aS)-4,4a-Dimethyl-6-(propan-2-ylidene)-4,4a,5,6,7,8-hexahydronaphthalen-2(3H)-o
	(-)-«beta»,«gamma»-Nootkatone
	«alpha»-Vetivone
	Isonootkatone
	(+)-«alpha»-Vetivone
	4«beta»H,5«alpha»-Eremophila-1(10),7(11)-dien-2-one
	(+)-Isonootkatone
	Vetiverone
	Isonootkaton
	(+)-«alpha»-Vetivon
	(4R-cis)-4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethylidene)naphthalen-2(3H)-o
Inchi:	InChI=1S/C15H22O/c1-10(2)12-5-6-13-8-14(16)7-11(3)15(13,4)9-12/h8,11H,5-7,9H2,1-4
InchiKey:	NIIPDXITZPFFTE-NHYWBVRUSA-N
Formula:	C15H22O
SMILES:	CC(C)=C1CCC2=CC(=O)CC(C)C2(C)C1
Mol. weight [g/mol]:	218.33
CAS:	15764-04-2

Physical Properties

Property code	Value	Unit	Source
gf	77.68	kJ/mol	Joback Method
hf	-241.88	kJ/mol	Joback Method
hfus	15.53	kJ/mol	Joback Method
hvap	54.42	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.048		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1813.00		NIST Webbook
rinpol	1813.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1845.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1851.00		NIST Webbook
rinpol	1842.00		NIST Webbook

rinpol	1809.00		NIST Webbook
tb	651.88	K	Joback Method
tc	891.67	K	Joback Method
tf	382.41	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.30	J/mol×K	651.88	Joback Method
cpg	560.66	J/mol×K	691.85	Joback Method
cpg	580.83	J/mol×K	731.81	Joback Method
cpg	599.99	J/mol×K	771.78	Joback Method
cpg	618.29	J/mol×K	811.74	Joback Method
cpg	635.88	J/mol×K	851.71	Joback Method
cpg	652.93	J/mol×K	891.67	Joback Method

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=C15764042&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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