.alpha.-Vetivone

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)C[C@@H](C)[C@@]2(C)C1
Mol. weight [g/mol]:	218.34

Physical Properties

Property code	Value	Unit	Source
hfus	15.53	kJ/mol	Joback Method
logp	4.048		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
rinpol	1825.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1845.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1813.00		NIST Webbook
rinpol	1813.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1851.00		NIST Webbook
rinpol	1842.00		NIST Webbook

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15764042&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices