

1,10-dihydronootkatone

Other names:	2(1H)-Naphthalenone, octahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R,8aS)- 4,4a-dimethyl-6-prop-1-en-2-yl-1,3,4,5,6,7,8,8a-octahydronaphthalen-2-one DIHIDRONOOTKATONE
Inchi:	InChI=1S/C15H24O/c1-10(2)12-5-6-13-8-14(16)7-11(3)15(13,4)9-12/h11-13H,1,5-9H2,2-
InchiKey:	NMALGKNZYKRHCE-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	C=C(C)C1CCC2CC(=O)CC(C)C2(C)C1
Mol. weight [g/mol]:	220.35
CAS:	20489-53-6

Physical Properties

Property code	Value	Unit	Source
gf	84.31	kJ/mol	Joback Method
hf	-279.47	kJ/mol	Joback Method
hfus	15.24	kJ/mol	Joback Method
hvap	51.39	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.984		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1766.00		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1766.00		NIST Webbook
ripol	2384.00		NIST Webbook
tb	628.44	K	Joback Method
tc	863.24	K	Joback Method
tf	348.53	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.28	J/molxK	628.44	Joback Method

cpg	587.52	J/mol×K	667.57	Joback Method
cpg	610.35	J/mol×K	706.71	Joback Method
cpg	631.90	J/mol×K	745.84	Joback Method
cpg	652.33	J/mol×K	784.97	Joback Method
cpg	671.78	J/mol×K	824.11	Joback Method
cpg	690.37	J/mol×K	863.24	Joback Method

Sources

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=C20489536&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	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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