1(2H)-Naphthalenone, octahydro-4a,8a-dimethyl-7-(1-methylethyl)-, [4aR-(4a«alpha»,7«beta», 8a«alpha»)]-

Other names:	1(2H)-Naphthalenone, octahydro-7«alpha»-isopropyl-4a«beta»,8a«beta»-dimethyl-, (+)- Jatamansone, (+)- Valeranone, (+)- (+)-Valeranone
Inchi:	InChI=1S/C15H26O/c1-11(2)12-7-9-14(3)8-5-6-13(16)15(14,4)10-12/h11-12H,5-10H2,1-4
InchiKey:	HDVXJTYHXDVWQO-UHFFFAOYSA-N
Formula:	C15H26O
SMILES:	CC(C)C1CCC2(C)CCCC(=O)C2(C)C1
Mol. weight [g/mol]:	222.37
CAS:	1803-39-0

Physical Properties

Property code	Value	Unit	Source
gf	4.80	kJ/mol	Joback Method
hf	-364.81	kJ/mol	Joback Method
hfus	6.94	kJ/mol	Joback Method
hvap	50.75	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	4.208		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1684.80		NIST Webbook
rinpol	1684.80		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1669.00		NIST Webbook
tb	636.35	K	Joback Method
tc	876.05	K	Joback Method
tf	377.39	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.33	J/mol×K	636.35	Joback Method

cpg	606.66	J/mol×K	676.30	Joback Method
cpg	629.73	J/mol×K	716.25	Joback Method
cpg	651.81	J/mol×K	756.20	Joback Method
cpg	673.17	J/mol×K	796.15	Joback Method
cpg	694.07	J/mol×K	836.10	Joback Method
cpg	714.79	J/mol×K	876.05	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=C1803390&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume