(2R,8R,8aS)-8,8a-Dimethyl-2-(prop-1-en-2-yl)-1,2,3

Other names:	Naphthalene, 1,2,6,7,8,8a-hexahydro-1,8a-dimethyl-7-(1-methylethenyl)-, (1R,7R,8aS)- 4«beta»H,5«alpha»-Eremophila-1,9,11-triene Naphthalene, 1,2,6,7,8,8a-hexahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1R-(1«alpha»,7«beta»,8a«alpha»)]- Nootkatene (-)-Nootkatene
Inchi:	InChI=1S/C15H22/c1-11(2)13-8-9-14-7-5-6-12(3)15(14,4)10-13/h5,7,9,12-13H,1,6,8,10H
InchiKey:	RSKODCFDTXJUBN-UHFFFAOYSA-N
Formula:	C15H22
SMILES:	C=C(C)C1CC=C2C=CCC(C)C2(C)C1
Mol. weight [g/mol]:	202.34
CAS:	5090-61-9

Physical Properties

Property code	Value	Unit	Source
gf	264.90	kJ/mol	Joback Method
hf	-17.34	kJ/mol	Joback Method
hfus	16.71	kJ/mol	Joback Method
hvap	48.69	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.501		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	1511.00		NIST Webbook
ripol	1815.00		NIST Webbook
tb	568.59	K	Joback Method
tc	795.68	K	Joback Method
tf	298.59	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.93	J/mol×K	568.59	Joback Method
cpg	502.32	J/mol×K	606.44	Joback Method

cpg	523.23	J/mol×K	644.29	Joback Method
cpg	542.85	J/mol×K	682.13	Joback Method
cpg	561.34	J/mol×K	719.98	Joback Method
cpg	578.86	J/mol×K	757.83	Joback Method
cpg	595.59	J/mol×K	795.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5090619&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

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