

2,2,9-Trimethyl-6-methylene-3,4,5,6,6a,7-hexahydro

Inchi:	InChI=1S/C15H22O/c1-10-5-7-12-9-15(16-14(12,3)4)11(2)6-8-13(10)15/h6,12-13H,1,5,7
InchiKey:	MGSOIRWVRUQEDG-RMTCENKZSA-N
Formula:	C15H22O
SMILES:	<chem>C=C1CCC2CC3(OC2(C)C)C(C)=CCC13</chem>
Mol. weight [g/mol]:	218.33

Physical Properties

Property code	Value	Unit	Source
gf	189.97	kJ/mol	Joback Method
hf	-144.32	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	52.25	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.857		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinsol	1554.00		NIST Webbook
tb	601.69	K	Joback Method
tc	834.50	K	Joback Method
tf	399.16	K	Joback Method
vc	0.709	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.87	J/mol×K	601.69	Joback Method
cpg	538.96	J/mol×K	640.49	Joback Method
cpg	558.72	J/mol×K	679.29	Joback Method
cpg	577.49	J/mol×K	718.10	Joback Method
cpg	595.55	J/mol×K	756.90	Joback Method
cpg	613.23	J/mol×K	795.70	Joback Method
cpg	630.83	J/mol×K	834.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407779&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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