

6-(1-Hydroxymethylvinyl)-4,8a-dimethyl-3,5,6,7,8,8a-octahydro-2H-chromene

Inchi:	InChI=1S/C15H22O2/c1-10-6-13(17)8-15(3)5-4-12(7-14(10)15)11(2)9-16/h12,16H,2,4-9H
InchiKey:	ZQMDPUQDUUCMDK-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	C=C(CO)C1CCC2(C)CC(=O)CC(C)=C2C1
Mol. weight [g/mol]:	234.33

Physical Properties

Property code	Value	Unit	Source
gf	-26.39	kJ/mol	Joback Method
hf	-356.18	kJ/mol	Joback Method
hfus	17.63	kJ/mol	Joback Method
hvap	70.30	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.021		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1909.00		NIST Webbook
rinpol	1909.00		NIST Webbook
tb	739.08	K	Joback Method
tc	959.07	K	Joback Method
tf	443.63	K	Joback Method
vc	0.750	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.38	J/mol×K	739.08	Joback Method
cpg	622.11	J/mol×K	775.74	Joback Method
cpg	639.08	J/mol×K	812.41	Joback Method
cpg	655.43	J/mol×K	849.07	Joback Method
cpg	671.28	J/mol×K	885.74	Joback Method
cpg	686.74	J/mol×K	922.40	Joback Method
cpg	701.94	J/mol×K	959.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U190514&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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