

Mint ketone (Salvial-4(14)-en-1-one)

Other names:	Savial-4(14)-en-1-one
Inchi:	InChI=1S/C14H22O/c1-9(2)11-5-6-12-13(11)8-10(3)4-7-14(12)15/h9,11-13H,3-8H2,1-2H
InchiKey:	KILBVQYCOPAGMH-PNESKVBLSA-N
Formula:	C14H22O
SMILES:	<chem>C=C1CCC(=O)C2CCC(C(C)C)C2C1</chem>
Mol. weight [g/mol]:	206.32

Physical Properties

Property code	Value	Unit	Source
gf	60.44	kJ/mol	Joback Method
hf	-290.41	kJ/mol	Joback Method
hfus	15.78	kJ/mol	Joback Method
hvap	50.98	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.594		Crippen Method
mcpvol	183.670	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1574.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1574.00		NIST Webbook
tb	612.15	K	Joback Method
tc	840.38	K	Joback Method
tf	332.00	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.61	J/molxK	612.15	Joback Method
cpg	533.60	J/molxK	650.19	Joback Method
cpg	555.21	J/molxK	688.23	Joback Method
cpg	575.44	J/molxK	726.27	Joback Method
cpg	594.33	J/molxK	764.30	Joback Method
cpg	611.89	J/molxK	802.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229811&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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