

Salvia-4(14),5-dien-1 «beta»-ol

Inchi:	InChI=1S/C14H22O/c1-9(2)11-5-6-12-13(11)8-10(3)4-7-14(12)15/h8-9,11-12,14-15H,3-7
InchiKey:	MKZJFJDDLDDOPO-SOGVLRHJSA-N
Formula:	C14H22O
SMILES:	C=C1C=C2C(C(C)C)CCC2C(O)CC1
Mol. weight [g/mol]:	206.32

Physical Properties

Property code	Value	Unit	Source
gf	66.54	kJ/mol	Joback Method
hf	-258.63	kJ/mol	Joback Method
hfus	21.20	kJ/mol	Joback Method
hvap	64.37	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.306		Crippen Method
mcvol	183.670	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	1605.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1605.00		NIST Webbook
tb	640.65	K	Joback Method
tc	843.36	K	Joback Method
tf	337.88	K	Joback Method
vc	0.683	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.48	J/molxK	640.65	Joback Method
cpg	539.80	J/molxK	674.44	Joback Method
cpg	557.07	J/molxK	708.22	Joback Method
cpg	573.31	J/molxK	742.01	Joback Method
cpg	588.58	J/molxK	775.79	Joback Method
cpg	602.90	J/molxK	809.58	Joback Method
cpg	616.31	J/molxK	843.36	Joback Method

dvisc	0.0057322	Paxs	337.88	Joback Method
dvisc	0.0020602	Paxs	388.34	Joback Method
dvisc	0.0009370	Paxs	438.80	Joback Method
dvisc	0.0005013	Paxs	489.26	Joback Method
dvisc	0.0003015	Paxs	539.73	Joback Method
dvisc	0.0001978	Paxs	590.19	Joback Method
dvisc	0.0001387	Paxs	640.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R201299&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
dvisc:	Dynamic viscosity
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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