Salviadienol

Inchi: InChI=1S/C15H24O/c1-10(2)12-7-8-15(4)13(12)9-11(3)5-6-14(15)16/h9-10,12,14,16H,3,5
InchiKey: JKYVXHLCMIJYEY-NWANDNLSSA-N
Formula: C15H24O
SMILES: C=C1C=C2C(C(C)C)CCC2(C)C(O)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
hfus	17.49	kJ/mol	Joback Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
ripol	2130.00		NIST Webbook
ripol	2130.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.06	J/mol×K	663.77	Joback Method
cpg	590.64	J/mol×K	698.22	Joback Method
cpg	608.29	J/mol×K	732.68	Joback Method
cpg	625.13	J/mol×K	767.13	Joback Method
cpg	641.29	J/mol×K	801.59	Joback Method
cpg	656.87	J/mol×K	836.04	Joback Method
cpg	671.99	J/mol×K	870.50	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R641300&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices