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-SNPRPXQTSA-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
rinpol	1549.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1549.00		NIST Webbook
ripol	2110.00		NIST Webbook
ripol	2110.00		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

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R420029&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

Legend

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