

(-)-trans-Selina-4(15),11-dien-5-ol

Inchi:	InChI=1S/C15H24O/c1-11(2)13-7-9-14(4)8-5-6-12(3)15(14,16)10-13/h13,16H,1,3,5-10H2
InchiKey:	OEFZSVXJENLPRM-GIJJTGMTSA-N
Formula:	C15H24O
SMILES:	<chem>C=C(C)C1CCC2(C)CCCC(=C)C2(O)C1</chem>
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	125.38	kJ/mol	Joback Method
hf	-174.18	kJ/mol	Joback Method
hfus	11.29	kJ/mol	Joback Method
hvap	63.14	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.840		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1629.00		NIST Webbook
rinpol	1629.00		NIST Webbook
tb	656.87	K	Joback Method
tc	871.41	K	Joback Method
tf	382.95	K	Joback Method
vc	0.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.87	J/mol×K	656.87	Joback Method
cpg	586.89	J/mol×K	692.63	Joback Method
cpg	605.07	J/mol×K	728.38	Joback Method
cpg	622.64	J/mol×K	764.14	Joback Method
cpg	639.81	J/mol×K	799.89	Joback Method
cpg	656.81	J/mol×K	835.65	Joback Method
cpg	673.87	J/mol×K	871.41	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R303038&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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