

Spirovetiva-3,7(11)-dien-12-ol

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H24O/c1-11(10-16)14-7-8-15(9-14)12(2)5-4-6-13(15)3/h5,13,16H,4,6-10H2

PINCZBXZNHNJMX-KAMYIIQDSA-N

C15H24O

CC1=CCCC(C)C12CCC(=C(C)CO)C2

220.35

Physical Properties

Property code	Value	Unit	Source
gf	63.45	kJ/mol	Joback Method
hf	-256.41	kJ/mol	Joback Method
hfus	20.11	kJ/mol	Joback Method
hvap	66.85	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.842		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1790.00		NIST Webbook
tb	676.24	K	Joback Method
tc	886.47	K	Joback Method
tf	375.01	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.61	J/mol×K	676.24	Joback Method
cpg	588.71	J/mol×K	711.28	Joback Method
cpg	605.93	J/mol×K	746.32	Joback Method
cpg	622.42	J/mol×K	781.36	Joback Method
cpg	638.30	J/mol×K	816.40	Joback Method
cpg	653.73	J/mol×K	851.43	Joback Method
cpg	668.83	J/mol×K	886.47	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R625635&Units=SI

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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