

2-Methoxyspirovetiva-2,4(15),7(11)-triene

Inchi:	InChI=1S/C16H24O/c1-11(2)14-6-7-16(10-14)12(3)8-15(17-5)9-13(16)4/h8,13H,3,6-7,9-
InchiKey:	MTLRUXVTDPIWGX-JBZHPUCOSA-N
Formula:	C16H24O
SMILES:	<chem>C=C1C=C(OC)CC(C)C12CCC(=C(C)C)C2</chem>
Mol. weight [g/mol]:	232.36

Physical Properties

Property code	Value	Unit	Source
gf	156.77	kJ/mol	Joback Method
hf	-172.80	kJ/mol	Joback Method
hfus	18.64	kJ/mol	Joback Method
hvap	54.96	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.619		Crippen Method
mcvol	207.550	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinsol	1693.00		NIST Webbook
tb	628.52	K	Joback Method
tc	850.41	K	Joback Method
tf	361.37	K	Joback Method
vc	0.783	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.23	J/mol×K	628.52	Joback Method
cpg	582.15	J/mol×K	665.50	Joback Method
cpg	601.94	J/mol×K	702.48	Joback Method
cpg	620.74	J/mol×K	739.47	Joback Method
cpg	638.68	J/mol×K	776.45	Joback Method
cpg	655.89	J/mol×K	813.43	Joback Method
cpg	672.53	J/mol×K	850.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R236047&Units=SI
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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