2-Methoxy-3,3-dimethylspirovetiva-1,4(15),7(11)-tr

Inchi: InChI=1S/C18H28O/c1-12(2)15-8-9-18(11-15)13(3)10-16(19-7)17(5,6)14(18)4/h10,13H,4
InchiKey: SWEORBGBXXGJKM-YJJYDOSJSA-N
Formula: C18H28O
SMILES: C=C1C(C)(C)C(OC)=CC(C)C12CCC(=C(C)C)C2
Mol. weight [g/mol]: 260.41

Physical Properties

Property code	Value	Unit	Source
gf	160.41	kJ/mol	Joback Method
hf	-219.18	kJ/mol	Joback Method
hfus	18.60	kJ/mol	Joback Method
hvap	57.95	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.255		Crippen Method
mcvol	235.730	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	1740.00		NIST Webbook
tb	669.85	K	Joback Method
tc	891.87	K	Joback Method
tf	403.57	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.05	J/mol×K	669.85	Joback Method
cpg	691.17	J/mol×K	706.85	Joback Method
cpg	712.42	J/mol×K	743.86	Joback Method
cpg	733.01	J/mol×K	780.86	Joback Method
cpg	753.18	J/mol×K	817.86	Joback Method
cpg	773.14	J/mol×K	854.86	Joback Method
cpg	793.14	J/mol×K	891.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R236032&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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