3,3-Dimethylspirovetiva-4(15),7(11)-dien-2-one

Inchi: InChI=1S/C17H26O/c1-11(2)14-7-8-17(10-14)12(3)9-15(18)16(5,6)13(17)4/h12H,4,7-10H
InchiKey: GVPVNMWWAQFAJO-MTATWXBHSA-N
Formula: C17H26O
SMILES: C=C1C(C)(C)C(=O)CC(C)C12CCC(=C(C)C)C2
Mol. weight [g/mol]: 246.39

Physical Properties

Property code	Value	Unit	Source
gf	114.07	kJ/mol	Joback Method
hf	-250.33	kJ/mol	Joback Method
hfus	13.49	kJ/mol	Joback Method
hvap	56.61	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.684		Crippen Method
mcvol	221.640	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinpol	1782.00		NIST Webbook
tb	688.23	K	Joback Method
tc	926.10	K	Joback Method
tf	425.01	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.57	J/mol×K	688.23	Joback Method
cpg	669.48	J/mol×K	727.88	Joback Method
cpg	691.54	J/mol×K	767.52	Joback Method
cpg	712.99	J/mol×K	807.17	Joback Method
cpg	734.09	J/mol×K	846.81	Joback Method
cpg	755.12	J/mol×K	886.46	Joback Method
cpg	776.33	J/mol×K	926.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R501445&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

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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