(1S ,1'R)-1-(6,6-dimethyl-bicyclo[3.1.1]hept-2-en-2-yl)-1-hydroxy-2-propanone (S)

Inchi: InChI=1S/C12H18O2/c1-7(13)11(14)9-5-4-8-6-10(9)12(8,2)3/h5,8,10-11,14H,4,6H2,1-3H

InchiKey: XMRUZCWDGKBXED-FBIMIBRVSA-N

Formula: C12H18O2

SMILES: CC(=O)C(O)C1=CCC2CC1C2(C)C

Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	-101.49	kJ/mol	Joback Method
hf	-380.45	kJ/mol	Joback Method
hfus	18.78	kJ/mol	Joback Method
hvap	64.83	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	1.929		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1383.00		NIST Webbook
ripol	2036.00		NIST Webbook
tb	637.03	K	Joback Method
tc	839.39	K	Joback Method
tf	386.05	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.88	J/mol×K	637.03	Joback Method
cpg	467.24	J/mol×K	670.76	Joback Method
cpg	480.86	J/mol×K	704.48	Joback Method
cpg	493.86	J/mol×K	738.21	Joback Method
cpg	506.35	J/mol×K	771.94	Joback Method
cpg	518.48	J/mol×K	805.67	Joback Method
cpg	530.37	J/mol×K	839.39	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=R522635&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume