(1S)-1-hydroxy-1-[(4'S)-4'-isopropenyl-1-cyclohexen-1-yl]-2-propanone (S)

InChI: InChI=1S/C12H18O2/c1-8(2)10-4-6-11(7-5-10)12(14)9(3)13/h6,10,12,14H,1,4-5,7H2,2-3

InChIKey: GALFHOWVRBFAIM-ZYHUDNBSSA-N

Formula: C12H18O2

SMILES: C=C(C)C1CC=C(C(O)C(C)=O)CC1

Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	-93.95	kJ/mol	Joback Method
hf	-344.83	kJ/mol	Joback Method
hfus	19.08	kJ/mol	Joback Method
hvap	66.14	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.239		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	1502.00		NIST Webbook
rinpol	1502.00		NIST Webbook
ripol	2197.00		NIST Webbook
ripol	2197.00		NIST Webbook
tb	639.82	K	Joback Method
tc	841.74	K	Joback Method
tf	325.69	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.81	J/mol×K	639.82	Joback Method
cpg	464.72	J/mol×K	673.47	Joback Method
cpg	478.75	J/mol×K	707.13	Joback Method
cpg	491.93	J/mol×K	740.78	Joback Method
cpg	504.30	J/mol×K	774.43	Joback Method
cpg	515.89	J/mol×K	808.09	Joback Method

cpg	526.73	J/mol×K	841.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R522655&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume