(1S,3S,5S)-1-Isopropyl-4-methylenebicyclo[3.1.0]h acetate

Inchi: InChI=1S/C12H18O2/c1-7(2)12-5-10(12)8(3)11(6-12)14-9(4)13/h7,10-11H,3,5-6H2,1-2,4
InchiKey: PBWRFXQNNGSAQG-QJPTWQEYSA-N
Formula: C12H18O2
SMILES: C=C1C(OC(C)=O)CC2(C(C)C)CC12
Mol. weight [g/mol]: 194.27
CAS: 139757-62-3

Physical Properties

Property code	Value	Unit	Source
gf	-24.82	kJ/mol	Joback Method
hf	-316.35	kJ/mol	Joback Method
hfus	15.98	kJ/mol	Joback Method
hvap	49.60	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.540		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	1297.00		NIST Webbook
tb	558.02	K	Joback Method
tc	764.52	K	Joback Method
tf	351.38	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.14	J/mol×K	558.02	Joback Method
cpg	433.79	J/mol×K	592.44	Joback Method
cpg	449.43	J/mol×K	626.85	Joback Method
cpg	464.18	J/mol×K	661.27	Joback Method
cpg	478.16	J/mol×K	695.68	Joback Method
cpg	491.51	J/mol×K	730.10	Joback Method
cpg	504.33	J/mol×K	764.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C139757623&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