2-((1R,4R)-4-Hydroxy-4-methylcyclohex-2-enyl)pro acetate

Inchi: InChI=1S/C12H20O3/c1-9(13)15-11(2,3)10-5-7-12(4,14)8-6-10/h5,7,10,14H,6,8H2,1-4H3

InchiKey: WMXMTKFKYOOQOL-ZYHUDNBSSA-N

Formula: C12H20O3

SMILES: CC(=O)OC(C)(C)C1C=CC(C)(O)CC1

Mol. weight [g/mol]: 212.29

CAS: 121958-61-0

Physical Properties

Property code	Value	Unit	Source
gf	-276.53	kJ/mol	Joback Method
hf	-589.79	kJ/mol	Joback Method
hfus	14.13	kJ/mol	Joback Method
hvap	66.11	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.045		Crippen Method
mcvol	178.090	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1457.40		NIST Webbook
tb	653.48	K	Joback Method
tc	859.50	K	Joback Method
tf	388.20	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.08	J/mol×K	653.48	Joback Method
cpg	516.74	J/mol×K	687.82	Joback Method
cpg	531.56	J/mol×K	722.15	Joback Method
cpg	545.65	J/mol×K	756.49	Joback Method
cpg	559.12	J/mol×K	790.82	Joback Method
cpg	572.07	J/mol×K	825.16	Joback Method
cpg	584.61	J/mol×K	859.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121958610&Units=SI

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