((1R,3R)-2,2-dimethyl-3-(2-methylprop-1-en-1-yl)cy
acetate

Inchi: InChI=1S/C12H20O2/c1-8(2)6-10-11(12(10,4)5)7-14-9(3)13/h6,10-11H,7H2,1-5H3/t10-,1

InchiKey: OTWVMTYIYNDIOQ-QWRGUYRKSA-N

Formula: C12H20O2

SMILES: CC(=O)OCC1C(C=C(C)C)C1(C)C

Mol. weight [g/mol]: 196.29

CAS: 54999-63-2

Physical Properties

Property code	Value	Unit	Source
gf	-72.25	kJ/mol	Joback Method
hf	-381.02	kJ/mol	Joback Method
hfus	22.49	kJ/mol	Joback Method
hvap	49.64	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.788		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	1285.50		NIST Webbook
tb	551.93	K	Joback Method
tc	750.39	K	Joback Method
tf	311.48	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.84	J/mol×K	551.93	Joback Method
cpg	449.74	J/mol×K	585.01	Joback Method
cpg	465.71	J/mol×K	618.08	Joback Method
cpg	480.85	J/mol×K	651.16	Joback Method
cpg	495.27	J/mol×K	684.24	Joback Method
cpg	509.05	J/mol×K	717.31	Joback Method
cpg	522.31	J/mol×K	750.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54999632&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume