1-Acetyl-4-isopropenyl-1-cyclopentene

Inchi: InChI=1S/C10H14O/c1-7(2)9-4-5-10(6-9)8(3)11/h5,9H,1,4,6H2,2-3H3
InchiKey: BTXSVMBTNJSALB-UHFFFAOYSA-N
Formula: C10H14O
SMILES: C=C(C)C1CC=C(C(C)=O)C1
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
gf	40.57	kJ/mol	Joback Method
hf	-139.88	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	45.22	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.488		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
ripol	1730.00		NIST Webbook
tb	498.05	K	Joback Method
tc	709.32	K	Joback Method
tf	260.85	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.67	J/mol×K	498.05	Joback Method
cpg	309.12	J/mol×K	533.26	Joback Method
cpg	323.69	J/mol×K	568.47	Joback Method
cpg	337.41	J/mol×K	603.68	Joback Method
cpg	350.32	J/mol×K	638.89	Joback Method
cpg	362.46	J/mol×K	674.10	Joback Method
cpg	373.86	J/mol×K	709.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R419346&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume