

Cyclopentane, 1-acetyl-3-isopropylidene

Inchi: InChI=1S/C10H16O/c1-7(2)9-4-5-10(6-9)8(3)11/h10H,4-6H2,1-3H3
InchiKey: QZHSUCSZBJSIEX-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC(=O)C1CCC(=C(C)C)C1
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	-22.14	kJ/mol	Joback Method
hf	-235.59	kJ/mol	Joback Method
hfus	16.20	kJ/mol	Joback Method
hvap	45.72	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.712		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
rinpol	1229.00		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1229.00		NIST Webbook
tb	503.87	K	Joback Method
tc	714.46	K	Joback Method
tf	259.69	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.63	J/molxK	503.87	Joback Method
cpg	328.11	J/molxK	538.97	Joback Method
cpg	343.68	J/molxK	574.07	Joback Method
cpg	358.36	J/molxK	609.16	Joback Method
cpg	372.21	J/molxK	644.26	Joback Method
cpg	385.24	J/molxK	679.36	Joback Method
cpg	397.51	J/molxK	714.46	Joback Method

Sources

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=R324768&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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