2-Acetylcyclopentanone

Other names: Acetylcyclopentanone
Cyclopentanone, 2-acetyl-
2-acetylcyclopentan-1-one
Inchi: InChI=1S/C7H10O2/c1-5(8)6-3-2-4-7(6)9/h6H,2-4H2,1H3
InchiKey: OSWDNIFICGLKEE-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CC(=O)C1CCCC1=O
Mol. weight [g/mol]: 126.15
CAS: 1670-46-8

Physical Properties

Property code	Value	Unit	Source
gf	-206.90	kJ/mol	Joback Method
hf	-377.61	kJ/mol	Joback Method
hfus	8.93	kJ/mol	Joback Method
hvap	42.43	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.945		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
tb	496.53	K	Joback Method
tc	722.38	K	Joback Method
tf	297.70	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.91	J/mol×K	496.53	Joback Method
cpg	237.74	J/mol×K	534.17	Joback Method
cpg	250.89	J/mol×K	571.81	Joback Method
cpg	263.36	J/mol×K	609.46	Joback Method
cpg	275.16	J/mol×K	647.10	Joback Method
cpg	286.26	J/mol×K	684.74	Joback Method

cpg	296.68	J/mol×K	722.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.70	K	1.00	NIST Webbook
tbrp	375.00 ± 1.00	K	3.20	NIST Webbook
tbrp	360.50 ± 2.50	K	2.00	NIST Webbook

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=C1670468&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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