

Cyclohexanone, 2-acetyl-

Other names:	«alpha»-Acetylcyclohexanone 2-Acetylcyclohexanone Acetylcyclohexanone 2-Acetyl-1-cyclohexanone
Inchi:	InChI=1S/C8H12O2/c1-6(9)7-4-2-3-5-8(7)10/h7H,2-5H2,1H3
InchiKey:	OEKATORRSPXJHE-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	CC(=O)C1CCCCC1=O
Mol. weight [g/mol]:	140.18
CAS:	874-23-7

Physical Properties

Property code	Value	Unit	Source
gf	-210.58	kJ/mol	Joback Method
hf	-404.41	kJ/mol	Joback Method
hfus	9.42	kJ/mol	Joback Method
hvap	44.82	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.335		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
ripol	1977.00		NIST Webbook
ripol	1977.00		NIST Webbook
tb	523.68	K	Joback Method
tc	754.10	K	Joback Method
tf	305.45	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.86	J/mol×K	523.68	Joback Method
cpg	283.80	J/mol×K	562.08	Joback Method
cpg	298.92	J/mol×K	600.49	Joback Method

cpg	313.22	J/mol×K	638.89	Joback Method
cpg	326.67	J/mol×K	677.29	Joback Method
cpg	339.27	J/mol×K	715.69	Joback Method
cpg	351.02	J/mol×K	754.10	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.70	K	2.40	NIST Webbook
tbrp	384.00	K	2.40	NIST Webbook
tbrp	389.00 ± 1.00	K	2.70	NIST Webbook
tbrp	368.00 ± 1.00	K	1.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C874237&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
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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