2-Cyclohexen-1-one, 3-methyl-

Other names:	Seudenone
	3-Methyl-2-cyclohexen-1-one
	3-Methyl-2-cyclohexene-1-one
	Methylcyclohexenone
	MCH
	3-Methyl-2-cyclohexenone
	3-methyl-2-cyclohexenone-1
	3-methylcyclohex-2-en-1-one
Inchi:	InChI=1S/C7H10O/c1-6-3-2-4-7(8)5-6/h5H,2-4H2,1H3
InchiKey:	IITQJMYAYSNIMI-UHFFFAOYSA-N
Formula:	C7H10O
SMILES:	CC1=CC(=O)CCC1
Mol. weight [g/mol]:	110.15
CAS:	1193-18-6

Physical Properties

Property code	Value	Unit	Source
gf	-62.04	kJ/mol	Joback Method
hf	-204.54	kJ/mol	Joback Method
hfus	4.99	kJ/mol	Joback Method
hvap	37.12	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.686		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
rinpol	1026.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1011.00		NIST Webbook
ripol	1577.00		NIST Webbook
ripol	1592.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1583.00		NIST Webbook
ripol	1592.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1579.00		NIST Webbook

ripol	1592.00		NIST Webbook
tb	472.70	K	NIST Webbook
tb	474.20	K	NIST Webbook
tc	683.63	K	Joback Method
tf	261.77	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.20	J/mol×K	455.74	Joback Method
cpg	202.73	J/mol×K	493.72	Joback Method
cpg	215.68	J/mol×K	531.70	Joback Method
cpg	228.03	J/mol×K	569.68	Joback Method
cpg	239.77	J/mol×K	607.66	Joback Method
cpg	250.90	J/mol×K	645.65	Joback Method
cpg	261.40	J/mol×K	683.63	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.50 ± 1.50	K	2.30	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1193186&Units=SI

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
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