2-Cyclohexen-1-one, 5-methyl-

Other names: 5-methyl-cyclohex-2-en-1-one
Inchi: InChI=1S/C7H10O/c1-6-3-2-4-7(8)5-6/h2,4,6H,3,5H2,1H3
InchiKey: NQICQYZVEPBJON-UHFFFAOYSA-N
Formula: C7H10O
SMILES: CC1CC=CC(=O)C1
Mol. weight [g/mol]: 110.15
CAS: 7214-50-8

Physical Properties

Property code	Value	Unit	Source
gf	-60.12	kJ/mol	Joback Method
hf	-213.41	kJ/mol	Joback Method
hfus	6.45	kJ/mol	Joback Method
hvap	36.14	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.542		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
rinpol	937.00		NIST Webbook
rinpol	970.00		NIST Webbook
ripol	1413.00		NIST Webbook
tb	446.09	K	Joback Method
tc	672.21	K	Joback Method
tf	245.01	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.41	J/mol×K	446.09	Joback Method
cpg	203.75	J/mol×K	483.78	Joback Method
cpg	217.47	J/mol×K	521.46	Joback Method
cpg	230.54	J/mol×K	559.15	Joback Method
cpg	242.97	J/mol×K	596.84	Joback Method

cpg	254.75	J/mol×K	634.53	Joback Method
cpg	265.87	J/mol×K	672.21	Joback Method

Sources

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=C7214508&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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