3-Methyl-3-cyclohexen-1-one

Other names: 3-Cyclohexen-1-one, 3-methyl-
3-Methylcyclohex-3-en-1-one
Inchi: InChI=1S/C7H10O/c1-6-3-2-4-7(8)5-6/h3H,2,4-5H2,1H3
InchiKey: MHBNXZDNKOXHCX-UHFFFAOYSA-N
Formula: C7H10O
SMILES: CC1=CCCC(=O)C1
Mol. weight [g/mol]: 110.15
CAS: 31883-98-4

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
tb	455.74	K	Joback Method
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

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=C31883984&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume