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

Inchi: InChI=1S/C7H10O/c1-6-4-2-3-5-7(6)8/h4H,2-3,5H2,1H3
InchiKey: LKTNAAYQZJAXCJ-UHFFFAOYSA-N
Formula: C7H10O
SMILES: CC1=CCCCC1=O
Mol. weight [g/mol]: 110.15
CAS: 1121-18-2

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	451.70	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	338.70	K	1.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1121182&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
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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