4-Hexen-2-one, 3-methyl-

Other names: 3-Methyl-4-hexen-2-one
Inchi: InChI=1S/C7H12O/c1-4-5-6(2)7(3)8/h4-6H,1-3H3/b5-4+
InchiKey: KXOKGQNYBFVWOX-SNAWJCMRSA-N
Formula: C7H12O
SMILES: CC=CC(C)C(C)=O
Mol. weight [g/mol]: 112.17
CAS: 72189-24-3

Physical Properties

Property code	Value	Unit	Source
gf	-43.08	kJ/mol	Joback Method
hf	-188.45	kJ/mol	Joback Method
hfus	12.16	kJ/mol	Joback Method
hvap	37.49	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.788		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
ripol	1260.00		NIST Webbook
ripol	1260.00		NIST Webbook
tb	417.15	K	Joback Method
tc	607.02	K	Joback Method
tf	198.50	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.13	J/mol×K	417.15	Joback Method
cpg	251.80	J/mol×K	575.38	Joback Method
cpg	242.50	J/mol×K	543.73	Joback Method
cpg	232.70	J/mol×K	512.09	Joback Method
cpg	222.38	J/mol×K	480.44	Joback Method
cpg	211.54	J/mol×K	448.80	Joback Method

cpg	260.64	J/mol×K	607.02	Joback Method
dvisc	0.0002393	Pa×s	417.15	Joback Method
dvisc	0.0003173	Pa×s	380.71	Joback Method
dvisc	0.0004467	Pa×s	344.27	Joback Method
dvisc	0.0006818	Pa×s	307.82	Joback Method
dvisc	0.0011658	Pa×s	271.38	Joback Method
dvisc	0.0023545	Pa×s	234.94	Joback Method
dvisc	0.0061552	Pa×s	198.50	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=C72189243&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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