4-Hexen-3-one, 5-methyl-

Other names: 5-Methyl-4-hexen-3-one
Inchi: InChI=1S/C7H12O/c1-4-7(8)5-6(2)3/h5H,4H2,1-3H3
InchiKey: WNZISGSGRPIJFX-UHFFFAOYSA-N
Formula: C7H12O
SMILES: CCC(=O)C=C(C)C
Mol. weight [g/mol]: 112.17
CAS: 13905-10-7

Physical Properties

Property code	Value	Unit	Source
gf	-49.19	kJ/mol	Joback Method
hf	-192.96	kJ/mol	Joback Method
hfus	14.38	kJ/mol	Joback Method
hvap	37.96	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.932		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
rinpol	1080.00		NIST Webbook
rinpol	1080.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1320.00		NIST Webbook
tb	417.47	K	Joback Method
tc	606.66	K	Joback Method
tf	199.54	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.06	J/mol×K	417.47	Joback Method
cpg	211.30	J/mol×K	449.00	Joback Method
cpg	221.99	J/mol×K	480.53	Joback Method
cpg	232.15	J/mol×K	512.07	Joback Method

cpg	241.82	J/mol×K	543.60	Joback Method
cpg	251.01	J/mol×K	575.13	Joback Method
cpg	259.74	J/mol×K	606.66	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=C13905107&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

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