6-Hepten-3-one, 4-methyl-

Other names: 4-Methyl-1-hepten-5-one
Inchi: InChI=1S/C8H14O/c1-4-6-7(3)8(9)5-2/h4,7H,1,5-6H2,2-3H3
InchiKey: AOXNCUPDNCMHRX-UHFFFAOYSA-N
Formula: C8H14O
SMILES: C=CCC(C)C(=O)CC
Mol. weight [g/mol]: 126.20
CAS: 26118-97-8

Physical Properties

Property code	Value	Unit	Source
gf	-27.04	kJ/mol	Joback Method
hf	-200.88	kJ/mol	Joback Method
hfus	13.27	kJ/mol	Joback Method
hvap	39.09	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.178		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
ripol	1113.00		NIST Webbook
ripol	1113.00		NIST Webbook
tb	432.55	K	Joback Method
tc	615.62	K	Joback Method
tf	213.09	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.57	J/mol×K	432.55	Joback Method
cpg	295.62	J/mol×K	585.10	Joback Method
cpg	285.43	J/mol×K	554.59	Joback Method
cpg	274.75	J/mol×K	524.08	Joback Method
cpg	263.55	J/mol×K	493.57	Joback Method
cpg	251.83	J/mol×K	463.06	Joback Method

cpg	305.33	J/mol×K	615.62	Joback Method
dvisc	0.0002805	Pa×s	432.55	Joback Method
dvisc	0.0003689	Pa×s	395.97	Joback Method
dvisc	0.0005129	Pa×s	359.40	Joback Method
dvisc	0.0007685	Pa×s	322.82	Joback Method
dvisc	0.0012767	Pa×s	286.24	Joback Method
dvisc	0.0024614	Pa×s	249.67	Joback Method
dvisc	0.0059449	Pa×s	213.09	Joback Method

Sources

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=C26118978&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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