Hept-6-en-2-one, 5-methyl

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

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
rinpol	988.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	982.00		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	251.83	J/mol×K	463.06	Joback Method
cpg	263.55	J/mol×K	493.57	Joback Method
cpg	274.75	J/mol×K	524.08	Joback Method
cpg	285.43	J/mol×K	554.59	Joback Method
cpg	295.62	J/mol×K	585.10	Joback Method

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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R419975&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
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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