3-hydroxy-pent-1-en-4-one

Inchi: InChI=1S/C5H8O2/c1-3-5(7)4(2)6/h3,5,7H,1H2,2H3
InchiKey: ZFTHRGXKSJKKCF-UHFFFAOYSA-N
Formula: C5H8O2
SMILES: C=CC(O)C(C)=O
Mol. weight [g/mol]: 100.12

Physical Properties

Property code	Value	Unit	Source
gf	-189.12	kJ/mol	Joback Method
hf	-291.19	kJ/mol	Joback Method
hfus	9.59	kJ/mol	Joback Method
hvap	49.09	kJ/mol	Joback Method
log10ws	-0.42		Crippen Method
logp	0.122		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
ripol	1381.00		NIST Webbook
ripol	1381.00		NIST Webbook
tb	456.09	K	Joback Method
tc	635.98	K	Joback Method
tf	240.10	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.78	J/mol×K	456.09	Joback Method
cpg	175.13	J/mol×K	486.07	Joback Method
cpg	182.14	J/mol×K	516.05	Joback Method
cpg	188.82	J/mol×K	546.04	Joback Method
cpg	195.18	J/mol×K	576.02	Joback Method
cpg	201.23	J/mol×K	606.00	Joback Method
cpg	206.98	J/mol×K	635.98	Joback Method
dvisc	0.0503690	Pa×s	240.10	Joback Method

dvisc	0.0115017	Pa×s	276.10	Joback Method
dvisc	0.0036926	Pa×s	312.10	Joback Method
dvisc	0.0014995	Pa×s	348.10	Joback Method
dvisc	0.0007210	Pa×s	384.09	Joback Method
dvisc	0.0003930	Pa×s	420.09	Joback Method
dvisc	0.0002358	Pa×s	456.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R241148&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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