4-hydroxymethylpentan-2-one

Other names: 4-(hydroxymethyl)-2-pentanone
Inchi: InChI=1S/C6H12O2/c1-5(4-7)3-6(2)8/h5,7H,3-4H2,1-2H3
InchiKey: NZBRXFKHZBOFBW-UHFFFAOYSA-N
Formula: C6H12O2
SMILES: CC(=O)CC(C)CO
Mol. weight [g/mol]: 116.16

Physical Properties

Property code	Value	Unit	Source
gf	-268.54	kJ/mol	Joback Method
hf	-437.26	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	51.99	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	0.594		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
rinpol	813.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	813.00		NIST Webbook
ripol	1374.00		NIST Webbook
ripol	1374.00		NIST Webbook
tb	482.29	K	Joback Method
tc	657.19	K	Joback Method
tf	253.13	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.83	J/mol×K	482.29	Joback Method
cpg	233.01	J/mol×K	511.44	Joback Method
cpg	241.81	J/mol×K	540.59	Joback Method
cpg	250.24	J/mol×K	569.74	Joback Method

cpg	258.31	J/mol×K	598.89	Joback Method
cpg	266.02	J/mol×K	628.04	Joback Method
cpg	273.38	J/mol×K	657.19	Joback Method
dvisc	0.0437428	Pa×s	253.13	Joback Method
dvisc	0.0098475	Pa×s	291.32	Joback Method
dvisc	0.0031323	Pa×s	329.52	Joback Method
dvisc	0.0012640	Pa×s	367.71	Joback Method
dvisc	0.0006050	Pa×s	405.90	Joback Method
dvisc	0.0003288	Pa×s	444.10	Joback Method
dvisc	0.0001967	Pa×s	482.29	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R60409&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume