2-Hexanone, 6-hydroxy-

Other names: 6-Hydroxy-hexan-2-one
Inchi: InChI=1S/C6H12O2/c1-6(8)4-2-3-5-7/h7H,2-5H2,1H3
InchiKey: UALYCKSVHDYQRP-UHFFFAOYSA-N
Formula: C6H12O2
SMILES: CC(=O)CCCCO
Mol. weight [g/mol]: 116.16
CAS: 21856-89-3

Physical Properties

Property code	Value	Unit	Source
gf	-266.10	kJ/mol	Joback Method
hf	-431.98	kJ/mol	Joback Method
hfus	16.98	kJ/mol	Joback Method
hvap	52.38	kJ/mol	Joback Method
log10ws	-0.88		Crippen Method
logp	0.738		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	500.20	K	NIST Webbook
tc	654.09	K	Joback Method
tf	268.13	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.60	J/mol×K	482.73	Joback Method
cpg	264.72	J/mol×K	625.53	Joback Method
cpg	257.18	J/mol×K	596.97	Joback Method
cpg	249.31	J/mol×K	568.41	Joback Method
cpg	241.09	J/mol×K	539.85	Joback Method
cpg	232.52	J/mol×K	511.29	Joback Method
cpg	271.93	J/mol×K	654.09	Joback Method
dvisc	0.0002069	Pa×s	482.73	Joback Method

dvisc	0.0003313	Pa×s	446.96	Joback Method
dvisc	0.0005759	Pa×s	411.20	Joback Method
dvisc	0.0011124	Pa×s	375.43	Joback Method
dvisc	0.0024680	Pa×s	339.66	Joback Method
dvisc	0.0066054	Pa×s	303.90	Joback Method
dvisc	0.0229887	Pa×s	268.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	385.20	K	2.00	NIST Webbook

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=C21856893&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume