

4-Hydroxy-3-hexanone

Other names:	3-Hexanone, 4-hydroxy- Ethyl «alpha»-hydroxypropyl ketone 3-Hydroxy-4-hexanone Propioin Propionoin 4-hydroxyhexan-3-one
Inchi:	InChI=1S/C6H12O2/c1-3-5(7)6(8)4-2/h5,7H,3-4H2,1-2H3
InchiKey:	SKCYVGUCBRYGTE-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCC(=O)C(O)CC
Mol. weight [g/mol]:	116.16
CAS:	4984-85-4

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	-0.99		Crippen Method
logp	0.736		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
rinpol	846.00		NIST Webbook
rinpol	846.00		NIST Webbook
tb	482.29	K	Joback Method
tc	657.19	K	Joback Method
tf	253.13	K	Joback Method
vc	0.391	m ³ /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/molxK	511.44	Joback Method
cpg	241.81	J/molxK	540.59	Joback Method
cpg	250.24	J/molxK	569.74	Joback Method
cpg	258.31	J/molxK	598.89	Joback Method
cpg	266.02	J/molxK	628.04	Joback Method
cpg	273.38	J/molxK	657.19	Joback Method
dvisc	0.0437428	Paxs	253.13	Joback Method
dvisc	0.0098475	Paxs	291.32	Joback Method
dvisc	0.0031323	Paxs	329.52	Joback Method
dvisc	0.0012640	Paxs	367.71	Joback Method
dvisc	0.0006050	Paxs	405.90	Joback Method
dvisc	0.0003288	Paxs	444.10	Joback Method
dvisc	0.0001967	Paxs	482.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	337.00 ± 1.00	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4984854&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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