

# 2-hexanon-3-ol

Inchi:	InChI=1S/C6H12O2/c1-3-4-6(8)5(2)7/h6,8H,3-4H2,1-2H3
InchiKey:	UHSBCAJZDUQTHH-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCCC(O)C(C)=O
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	-0.99		Crippen Method
logp	0.736		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
ripol	1430.00		NIST Webbook
ripol	1430.00		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/molxK	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

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R240907&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R240907&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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