

# 3-Hexanol, 4-ethyl-

Other names:	4-Ethyl-3-hexanol
Inchi:	InChI=1S/C8H18O/c1-4-7(5-2)8(9)6-3/h7-9H,4-6H2,1-3H3
InchiKey:	BOJLCKCCKQMGKD-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCC(O)C(CC)CC
Mol. weight [g/mol]:	130.23
CAS:	19780-44-0

## Physical Properties

Property code	Value	Unit	Source
gf	-125.22	kJ/mol	Joback Method
hf	-371.24	kJ/mol	Joback Method
hfus	13.52	kJ/mol	Joback Method
hvap	49.31	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.194		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	953.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	953.00		NIST Webbook
tb	438.15 ± 5.00	K	NIST Webbook
tb	436.15 ± 3.00	K	NIST Webbook
tc	639.93	K	Joback Method
tf	210.74	K	Joback Method
vc	0.490	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.39	J/mol×K	473.74	Joback Method
cpg	302.54	J/mol×K	501.44	Joback Method
cpg	314.22	J/mol×K	529.14	Joback Method
cpg	325.44	J/mol×K	556.84	Joback Method

cpg	336.21	J/mol×K	584.53	Joback Method
cpg	346.54	J/mol×K	612.23	Joback Method
cpg	356.45	J/mol×K	639.93	Joback Method
dvisc	0.3001577	Paxs	210.74	Joback Method
dvisc	0.0290327	Paxs	254.57	Joback Method
dvisc	0.0055777	Paxs	298.41	Joback Method
dvisc	0.0016351	Paxs	342.24	Joback Method
dvisc	0.0006333	Paxs	386.07	Joback Method
dvisc	0.0002977	Paxs	429.91	Joback Method
dvisc	0.0001609	Paxs	473.74	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.65596e+01
Coeff. B	-4.65790e+03
Coeff. C	-4.60840e+01
Temperature range (K), min.	332.34
Temperature range (K), max.	460.19

## Sources

**The Yaws Handbook of Vapor Pressure:**  
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>  
<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/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=C19780440&Units=SI>

## Legend

**cpg:** Ideal gas heat capacity  
**dvisc:** Dynamic viscosity  
**gf:** 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>pvap:</b>	Vapor pressure
<b>rinpola:</b>	Non-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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