

# 2-Heptanol, 5-methyl-

<b>Other names:</b>	5-Methyl-2-heptanol
<b>Inchi:</b>	InChI=1S/C8H18O/c1-4-7(2)5-6-8(3)9/h7-9H,4-6H2,1-3H3
<b>InchiKey:</b>	FYMBAYNKBWGEIK-UHFFFAOYSA-N
<b>Formula:</b>	C8H18O
<b>SMILES:</b>	CCC(C)CCC(C)O
<b>Mol. weight [g/mol]:</b>	130.23
<b>CAS:</b>	54630-50-1

## 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	856.00		NIST Webbook
ripol	1394.00		NIST Webbook
ripol	1395.00		NIST Webbook
tb	445.05 ± 0.50	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	356.45	J/mol×K	639.93	Joback Method
cpg	346.54	J/mol×K	612.23	Joback Method
cpg	336.21	J/mol×K	584.53	Joback Method
cpg	325.44	J/mol×K	556.84	Joback Method
cpg	314.22	J/mol×K	529.14	Joback Method

cpg	302.54	J/mol×K	501.44	Joback Method
cpg	290.39	J/mol×K	473.74	Joback Method
cpl	296.20	J/mol×K	298.50	NIST Webbook
dvisc	0.0001609	Paxs	473.74	Joback Method
dvisc	0.3001577	Paxs	210.74	Joback Method
dvisc	0.0002977	Paxs	429.91	Joback Method
dvisc	0.0006333	Paxs	386.07	Joback Method
dvisc	0.0016351	Paxs	342.24	Joback Method
dvisc	0.0055777	Paxs	298.41	Joback Method
dvisc	0.0290327	Paxs	254.57	Joback Method
hvapt	47.20	kJ/mol	396.50	NIST Webbook
hvapt	51.90	kJ/mol	396.50	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.67459e+01
Coeff. B	-4.99895e+03
Coeff. C	-3.28520e+01
Temperature range (K), min.	336.59
Temperature range (K), max.	470.04

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C54630501&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54630501&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>

## Legend

**cpg:** Ideal gas heat capacity

<b>cpl:</b>	Liquid phase 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>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</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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