

2-Heptanol, 2-methyl-

Other names:	2-Methyl-2-heptanol 2-methylheptan-2-ol dimethylpentylcarbinol
Inchi:	InChI=1S/C8H18O/c1-4-5-6-7-8(2,3)9/h9H,4-7H2,1-3H3
InchiKey:	ACBMYVZWKYLP-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCCCC(C)(C)O
Mol. weight [g/mol]:	130.23
CAS:	625-25-2

Physical Properties

Property code	Value	Unit	Source
gf	-117.50	kJ/mol	Joback Method
hf	-369.43	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	62.90 ± 0.20	kJ/mol	NIST Webbook
log10ws	-1.72		Estimated Solubility Method
log10ws	-1.72		Aqueous Solubility Prediction Method
logp	2.338		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
rinpol	919.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	879.90		NIST Webbook
rinpol	920.00		NIST Webbook
ripol	1280.00		NIST Webbook
ripol	1265.00		NIST Webbook

tb	471.39	K	Joback Method
tc	640.25	K	Joback Method
tf	222.95	K	Aqueous Solubility Prediction Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.85	J/mol×K	471.39	Joback Method
cpg	305.37	J/mol×K	499.53	Joback Method
cpg	317.32	J/mol×K	527.68	Joback Method
cpg	328.71	J/mol×K	555.82	Joback Method
cpg	339.57	J/mol×K	583.96	Joback Method
cpg	349.91	J/mol×K	612.10	Joback Method
cpg	359.77	J/mol×K	640.25	Joback Method
cpl	337.60	J/mol×K	298.50	NIST Webbook
dvisc	0.0742698	Pa×s	243.16	Joback Method
dvisc	0.0138116	Pa×s	281.20	Joback Method
dvisc	0.0038351	Pa×s	319.24	Joback Method
dvisc	0.0013989	Pa×s	357.27	Joback Method
dvisc	0.0006196	Pa×s	395.31	Joback Method
dvisc	0.0003166	Pa×s	433.35	Joback Method
dvisc	0.0001803	Pa×s	471.39	Joback Method
hvapt	55.00	kJ/mol	384.00	NIST Webbook
hvapt	53.10	kJ/mol	386.50	NIST Webbook
pvap	0.01	kPa	275.40	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols

pvap	0.02	kPa	278.40	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.02	kPa	281.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.03	kPa	284.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.04	kPa	287.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols

pvap	0.05	kPa	290.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.06	kPa	293.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.08	kPa	296.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.11	kPa	299.30	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols

pvap	0.14	kPa	302.30	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.18	kPa	305.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.23	kPa	308.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
pvap	0.28	kPa	311.30	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols

pvap	0.35	kPa	314.20	Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols
------	------	-----	--------	--

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	340.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49721e+01
Coeff. B	-3.48722e+03
Coeff. C	-9.51910e+01
Temperature range (K), min.	332.67
Temperature range (K), max.	456.17

Sources

Crippen Method:
Measurement and Prediction of Thermochemical Properties. Improved Benson-Type Increments for the Estimation of Enthalpies of Vaporization and Standard Enthalpies of Formation of Aliphatic Alcohols:
Estimated Solubility Method:
McGowan Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>
<https://www.doi.org/10.1021/je049561m>
https://en.wikipedia.org/wiki/Joback_method
<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>
http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C625252&Units=SI>

The Yaws Handbook of Vapor
Pressure:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	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

Latest version available from:

<https://www.chemeo.com/cid/15-388-5/2-Heptanol-2-methyl.pdf>

Generated by Cheméo on 2025-12-05 10:04:54.380197756 +0000 UTC m=+4677291.910238409.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.