

2-methyl-1-hexanol

Other names:	1-Hexanol, 2-methyl- 2-methylhexan-1-ol
Inchi:	InChI=1S/C7H16O/c1-3-4-5-7(2)6-8/h7-8H,3-6H2,1-2H3
InchiKey:	LCFKURIJYIJNRU-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCCC(C)CO
Mol. weight [g/mol]:	116.20
CAS:	624-22-6

Physical Properties

Property code	Value	Unit	Source
gf	-131.20	kJ/mol	Joback Method
hf	-345.32	kJ/mol	Joback Method
hfus	14.45	kJ/mol	Joback Method
hvap	47.47	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.805		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpola	886.00		NIST Webbook
rinpola	886.00		NIST Webbook
rinpola	915.00		NIST Webbook
tb	437.65 ± 2.00	K	NIST Webbook
tb	436.00 ± 4.00	K	NIST Webbook
tb	436.85 ± 0.50	K	NIST Webbook
tc	615.06	K	Joback Method
tf	214.47	K	Joback Method
vc	0.441	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.92	J/mol×K	451.30	Joback Method
cpg	258.79	J/mol×K	478.59	Joback Method

cpg	269.25	J/molxK	505.89	Joback Method
cpg	279.32	J/molxK	533.18	Joback Method
cpg	289.00	J/molxK	560.47	Joback Method
cpg	298.30	J/molxK	587.77	Joback Method
cpg	307.23	J/molxK	615.06	Joback Method
dvisc	0.1594974	Paxs	214.47	Joback Method
dvisc	0.0221021	Paxs	253.94	Joback Method
dvisc	0.0052125	Paxs	293.41	Joback Method
dvisc	0.0017316	Paxs	332.88	Joback Method
dvisc	0.0007266	Paxs	372.36	Joback Method
dvisc	0.0003601	Paxs	411.83	Joback Method
dvisc	0.0002018	Paxs	451.30	Joback Method
hvapt	53.50	kJ/mol	390.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56404e+01
Coeff. B	-3.81411e+03
Coeff. C	-8.99570e+01
Temperature range (K), min.	338.39
Temperature range (K), max.	459.22

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C624226&Units=SI>

The Yaws Handbook of Vapor Pressure:

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

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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
hvac:	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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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