1-Hexanol, 4-methyl-

Other names:	4-Methyl-1-hexanol
	4-Methylhexan-1-ol
	4-Methylhexanol
Inchi:	InChI=1S/C7H16O/c1-3-7(2)5-4-6-8/h7-8H,3-6H2,1-2H3
InchiKey:	YNPVNLWKVZZBTM-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCC(C)CCCO
Mol. weight [g/mol]:	116.20
CAS:	818-49-5

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
rinpol	955.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	925.90		NIST Webbook
rinpol	925.90		NIST Webbook
rinpol	925.90		NIST Webbook
rinpol	950.00		NIST Webbook
ripol	1434.00		NIST Webbook
ripol	1445.00		NIST Webbook
ripol	1443.00		NIST Webbook
ripol	1434.00		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1414.00		NIST Webbook
tb	446.15 ± 1.00	K	NIST Webbook
tb	436.15 ± 2.00	K	NIST Webbook
tc	615.06	K	Joback Method
tf	214.47	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.23	J/mol×K	615.06	Joback Method
cpg	247.92	J/mol×K	451.30	Joback Method
cpg	258.79	J/mol×K	478.59	Joback Method
cpg	269.25	J/mol×K	505.89	Joback Method
cpg	279.32	J/mol×K	533.18	Joback Method
cpg	289.00	J/mol×K	560.47	Joback Method
cpg	298.30	J/mol×K	587.77	Joback Method
dvisc	0.0002018	Pa×s	451.30	Joback Method
dvisc	0.1594974	Pa×s	214.47	Joback Method
dvisc	0.0221021	Pa×s	253.94	Joback Method
dvisc	0.0052125	Pa×s	293.41	Joback Method
dvisc	0.0017316	Pa×s	332.88	Joback Method
dvisc	0.0007266	Pa×s	372.36	Joback Method
dvisc	0.0003601	Pa×s	411.83	Joback Method
hvapt	62.60	kJ/mol	398.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51728e+01
Coeff. B	-3.55282e+03
Coeff. C	-1.09531e+02
Temperature range (K), min.	348.21
Temperature range (K), max.	469.81

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C818495&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume