1-Hexanol, 3-methyl-

Other names: 3-Methyl-1-hexanol
3-Methylhexan-1-ol
3-Methylhexanol
Inchi: InChI=1S/C7H16O/c1-3-4-7(2)5-6-8/h7-8H,3-6H2,1-2H3
InchiKey: YGZVAQICDGBHMD-UHFFFAOYSA-N
Formula: C7H16O
SMILES: CCCC(C)CCO
Mol. weight [g/mol]: 116.20
CAS: 13231-81-7

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	895.00		NIST Webbook
rinpol	895.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1413.00		NIST Webbook
tb	445.35 ± 0.30	K	NIST Webbook
tb	445.35 ± 0.50	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	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
cpg	307.23	J/mol×K	615.06	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
dvisc	0.0002018	Pa×s	451.30	Joback Method
hvapt	57.40	kJ/mol	399.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50588e+01
Coeff. B	-3.46319e+03
Coeff. C	-1.13641e+02
Temperature range (K), min.	348.10
Temperature range (K), max.	468.94

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13231817&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
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