3-Hexanol, 4-methyl-

Other names: 2-Ethyl-3-pentanol
3-Methyl-4-hexanol
3-Pentanol, 2-ethyl-
4-Methyl-3-hexanol
4-Methylhexan-3-ol
Inchi: InChI=1S/C7H16O/c1-4-6(3)7(8)5-2/h6-8H,4-5H2,1-3H3
InchiKey: NZPGYIBESMMUFU-UHFFFAOYSA-N
Formula: C7H16O
SMILES: CCC(C)C(O)CC
Mol. weight [g/mol]: 116.20
CAS: 615-29-2

Physical Properties

Property code	Value	Unit	Source
gf	-133.64	kJ/mol	Joback Method
hf	-350.60	kJ/mol	Joback Method
hfus	10.93	kJ/mol	Joback Method
hvap	47.08	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.803		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	721.00		NIST Webbook
rinpol	721.00		NIST Webbook
ripol	1583.00		NIST Webbook
tb	422.65 ± 3.00	K	NIST Webbook
tc	618.05	K	Joback Method
tf	199.47	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.03	J/mol×K	450.86	Joback Method

cpg	299.70	J/mol×K	590.19	Joback Method
cpg	290.18	J/mol×K	562.32	Joback Method
cpg	280.27	J/mol×K	534.46	Joback Method
cpg	269.95	J/mol×K	506.59	Joback Method
cpg	259.20	J/mol×K	478.73	Joback Method
cpg	308.82	J/mol×K	618.05	Joback Method
dvisc	0.0001931	Pa×s	450.86	Joback Method
dvisc	0.0003619	Pa×s	408.96	Joback Method
dvisc	0.0007829	Pa×s	367.06	Joback Method
dvisc	0.0020664	Pa×s	325.16	Joback Method
dvisc	0.0072680	Pa×s	283.27	Joback Method
dvisc	0.0395574	Pa×s	241.37	Joback Method
dvisc	0.4386858	Pa×s	199.47	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.72599e+01
Coeff. B	-5.34105e+03
Coeff. C	-1.50000e-01
Temperature range (K), min.	314.84
Temperature range (K), max.	447.16

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C615292&Units=SI

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
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