3-Hexanol, 5-methyl-

Other names: 5-Methyl-3-hexanol
Inchi: InChI=1S/C7H16O/c1-4-7(8)5-6(2)3/h6-8H,4-5H2,1-3H3
InchiKey: RGCZULIFYUPTAR-UHFFFAOYSA-N
Formula: C7H16O
SMILES: CCC(O)CC(C)C
Mol. weight [g/mol]: 116.20
CAS: 623-55-2

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	59.80 ± 0.30	kJ/mol	NIST Webbook
log10ws	-1.89		Crippen Method
logp	1.803		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	838.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	838.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1262.00		NIST Webbook
tb	420.15 ± 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	308.82	J/mol×K	618.05	Joback Method
cpg	259.20	J/mol×K	478.73	Joback Method

cpg	269.95	J/mol×K	506.59	Joback Method
cpg	280.27	J/mol×K	534.46	Joback Method
cpg	290.18	J/mol×K	562.32	Joback Method
cpg	299.70	J/mol×K	590.19	Joback Method
cpg	248.03	J/mol×K	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	0.0001931	Pa×s	450.86	Joback Method
dvisc	0.4386858	Pa×s	199.47	Joback Method
pvap	0.18	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	0.23	kPa	299.20	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	0.29	kPa	302.20	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	0.37	kPa	305.30	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	0.46	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	0.57	kPa	311.20	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	0.10	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	0.08	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	0.06	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	0.05	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	0.04	kPa	278.20	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	275.20	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	0.14	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.66686e+01
Coeff. B	-4.64088e+03
Coeff. C	-3.50230e+01
Temperature range (K), min.	318.33
Temperature range (K), max.	443.66

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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:	https://www.doi.org/10.1021/je049561m
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=C623552&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
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