

2-Hexanol, 3-methyl-

Other names:	3-Methyl-2-hexanol 3-methylhexan-2-ol
Inchi:	InChI=1S/C7H16O/c1-4-5-6(2)7(3)8/h6-8H,4-5H2,1-3H3
InchiKey:	IRLSKJITMWPWNY-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCC(C)C(C)O
Mol. weight [g/mol]:	116.20
CAS:	2313-65-7

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	909.00		NIST Webbook
rinpol	906.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1331.00		NIST Webbook
tb	424.65 ± 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	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	308.82	J/mol×K	618.05	Joback Method
dvisc	0.4386858	Pa×s	199.47	Joback Method
dvisc	0.0395574	Pa×s	241.37	Joback Method
dvisc	0.0072680	Pa×s	283.27	Joback Method
dvisc	0.0020664	Pa×s	325.16	Joback Method
dvisc	0.0007829	Pa×s	367.06	Joback Method
dvisc	0.0003619	Pa×s	408.96	Joback Method
dvisc	0.0001931	Pa×s	450.86	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.65488e+01
Coeff. B	-4.61151e+03
Coeff. C	-3.81190e+01
Temperature range (K), min.	321.71
Temperature range (K), max.	448.49

Sources

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=C2313657&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/ci990307I

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

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