4-Methyl-2-hexanol

Inchi: InChI=1S/C7H16O/c1-4-6(2)5-7(3)8/h6-8H,4-5H2,1-3H3
InchiKey: KZUBXUKRWLMPIO-UHFFFAOYSA-N
Formula: C7H16O
SMILES: CCC(C)CC(C)O
Mol. weight [g/mol]: 116.20
CAS: 2313-61-3

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
tb	423.65 ± 1.50	K	NIST Webbook
tb	425.15 ± 2.00	K	NIST Webbook
tb	421.15 ± 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	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	1.49498e+01
Coeff. B	-3.06775e+03
Coeff. C	-1.24217e+02
Temperature range (K), min.	333.45
Temperature range (K), max.	442.50

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2313613&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume