2-Hexanol, 3,4-dimethyl-

Other names: 3,4-Dimethyl-2-hexanol
Inchi: InChI=1S/C8H18O/c1-5-6(2)7(3)8(4)9/h6-9H,5H2,1-4H3
InchiKey: LBJWJHMCZHKLQU-UHFFFAOYSA-N
Formula: C8H18O
SMILES: CCC(C)C(C)C(C)O
Mol. weight [g/mol]: 130.23
CAS: 19550-05-1

Physical Properties

Property code	Value	Unit	Source
gf	-127.66	kJ/mol	Joback Method
hf	-376.52	kJ/mol	Joback Method
hfus	9.99	kJ/mol	Joback Method
hvap	48.92	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.049		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	473.30	K	Joback Method
tc	642.89	K	Joback Method
tf	195.74	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.54	J/mol×K	473.30	Joback Method
cpg	348.04	J/mol×K	614.62	Joback Method
cpg	337.49	J/mol×K	586.36	Joback Method
cpg	326.48	J/mol×K	558.09	Joback Method
cpg	314.99	J/mol×K	529.83	Joback Method
cpg	303.02	J/mol×K	501.56	Joback Method
cpg	358.15	J/mol×K	642.89	Joback Method
dvisc	0.0001533	Pa×s	473.30	Joback Method

dvisc	0.0002974	Pa×s	427.04	Joback Method
dvisc	0.0006781	Pa×s	380.78	Joback Method
dvisc	0.0019417	Pa×s	334.52	Joback Method
dvisc	0.0077930	Pa×s	288.26	Joback Method
dvisc	0.0532070	Pa×s	242.00	Joback Method
dvisc	0.9006667	Pa×s	195.74	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.72814e+01
Coeff. B	-5.62191e+03
Coeff. C	-1.50000e-01
Temperature range (K), min.	330.97
Temperature range (K), max.	469.82

Sources

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=C19550051&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume