3-Hexanol, 3,5-dimethyl-

Other names: 3,5-Dimethyl-3-hexanol
3,5-dimethylhexan-3-ol
Inchi: InChI=1S/C8H18O/c1-5-8(4,9)6-7(2)3/h7,9H,5-6H2,1-4H3
InchiKey: INMGJWCKWKKMPN-UHFFFAOYSA-N
Formula: C8H18O
SMILES: CCC(C)(O)CC(C)C
Mol. weight [g/mol]: 130.23
CAS: 4209-91-0

Physical Properties

Property code	Value	Unit	Source
gf	-119.94	kJ/mol	Joback Method
hf	-374.71	kJ/mol	Joback Method
hfus	9.63	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.194		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	883.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	883.00		NIST Webbook
tb	470.95	K	Joback Method
tc	643.32	K	Joback Method
tf	228.16	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.99	J/mol×K	470.95	Joback Method
cpg	305.85	J/mol×K	499.68	Joback Method
cpg	318.10	J/mol×K	528.41	Joback Method
cpg	329.77	J/mol×K	557.13	Joback Method

cpg	340.87	J/mol×K	585.86	Joback Method
cpg	351.43	J/mol×K	614.59	Joback Method
cpg	361.48	J/mol×K	643.32	Joback Method
dvisc	0.1736472	Pa×s	228.16	Joback Method
dvisc	0.0230030	Pa×s	268.62	Joback Method
dvisc	0.0051732	Pa×s	309.09	Joback Method
dvisc	0.0016435	Pa×s	349.55	Joback Method
dvisc	0.0006624	Pa×s	390.02	Joback Method
dvisc	0.0003167	Pa×s	430.49	Joback Method
dvisc	0.0001719	Pa×s	470.95	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.69503e+01
Coeff. B	-5.18598e+03
Coeff. C	-4.96700e+00
Temperature range (K), min.	316.20
Temperature range (K), max.	450.54

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=C4209910&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume