3-Hexanol, 2,2-dimethyl-

Other names:	2,2-Dimethyl-3-hexanol
	2,2-dimethylhexan-3-ol
	n-Propyl-tert-butylcarbinoll
Inchi:	InChI=1S/C8H18O/c1-5-6-7(9)8(2,3)4/h7,9H,5-6H2,1-4H3
InchiKey:	PFHLGQKVKALLMD-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCCC(O)C(C)(C)C
Mol. weight [g/mol]:	130.23
CAS:	4209-90-9

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	906.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	906.00		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	351.43	J/mol×K	614.59	Joback Method
cpg	340.87	J/mol×K	585.86	Joback Method
cpg	329.77	J/mol×K	557.13	Joback Method
cpg	318.10	J/mol×K	528.41	Joback Method
cpg	305.85	J/mol×K	499.68	Joback Method
cpg	361.48	J/mol×K	643.32	Joback Method
dvisc	0.0001719	Pa×s	470.95	Joback Method
dvisc	0.0003167	Pa×s	430.49	Joback Method
dvisc	0.0006624	Pa×s	390.02	Joback Method
dvisc	0.0016435	Pa×s	349.55	Joback Method
dvisc	0.0051732	Pa×s	309.09	Joback Method
dvisc	0.0230030	Pa×s	268.62	Joback Method
dvisc	0.1736472	Pa×s	228.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.89249e+01
Coeff. B	-6.45844e+03
Coeff. C	3.14330e+01
Temperature range (K), min.	315.10
Temperature range (K), max.	442.99

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

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