3-Pentanol, 2,2-dimethyl-

Other names:	2,2-Dimethyl-3-pentanol
	2,2-dimethylpentan-3-ol
Inchi:	InChI=1S/C7H16O/c1-5-6(8)7(2,3)4/h6,8H,5H2,1-4H3
InchiKey:	HMSVXZJWPVIVIV-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCC(O)C(C)(C)C
Mol. weight [g/mol]:	116.20
CAS:	3970-62-5

Physical Properties

Property code	Value	Unit	Source
gf	-128.36	kJ/mol	Joback Method
hf	-354.07	kJ/mol	Joback Method
hfus	7.04	kJ/mol	Joback Method
hvap	46.17	kJ/mol	Joback Method
log10ws	-1.15		Aqueous Solubility Prediction Method
logp	1.803		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
rinpol	814.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	814.00		NIST Webbook
tb	448.07	K	Joback Method
tc	621.71	K	Joback Method
tf	271.48	K	Aqueous Solubility Prediction Method
tf	280.50	K	Calorimetric and FTIR study of selected aliphatic heptanols
tf	282.45 ± 0.50	K	NIST Webbook
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.49	J/mol×K	448.07	Joback Method
cpg	262.44	J/mol×K	477.01	Joback Method
cpg	273.81	J/mol×K	505.95	Joback Method
cpg	284.62	J/mol×K	534.89	Joback Method
cpg	294.91	J/mol×K	563.83	Joback Method
cpg	304.69	J/mol×K	592.77	Joback Method
cpg	313.99	J/mol×K	621.71	Joback Method
dvisc	0.2459675	Pa×s	216.89	Joback Method
dvisc	0.0312263	Pa×s	255.42	Joback Method
dvisc	0.0068100	Pa×s	293.95	Joback Method
dvisc	0.0021138	Pa×s	332.48	Joback Method
dvisc	0.0008366	Pa×s	371.01	Joback Method
dvisc	0.0003942	Pa×s	409.54	Joback Method
dvisc	0.0002114	Pa×s	448.07	Joback Method
hvapt	51.40	kJ/mol	364.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49725e+01
Coeff. B	-3.25877e+03
Coeff. C	-9.42700e+01
Temperature range (K), min.	316.18
Temperature range (K), max.	431.58

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3970625&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
Calorimetric and FTIR study of selected aliphatic heptanols:	https://www.doi.org/10.1016/j.fluid.2016.04.003

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
hvapt:	Enthalpy of vaporization at a given temperature
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