3-Pentanol, 2-methyl-

Other names:	2-Methyl-3-pentanol
	2-methylpentan-3-ol
	4-Methyl-3-pentanol
	Propanol, 1-isopropyl-
Inchi:	InChI=1S/C6H14O/c1-4-6(7)5(2)3/h5-7H,4H2,1-3H3
InchiKey:	ISTJMQSHILQAEC-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CCC(O)C(C)C
Mol. weight [g/mol]:	102.17
CAS:	565-67-3

Physical Properties

Property code	Value	Unit	Source
gf	-142.06	kJ/mol	Joback Method
hf	-338.90 ± 2.20	kJ/mol	NIST Webbook
hfl	-396.40 ± 1.00	kJ/mol	NIST Webbook
hfus	8.34	kJ/mol	Joback Method
hvap	56.00 ± 0.50	kJ/mol	NIST Webbook
log10ws	-0.70		Estimated Solubility Method
log10ws	-0.70		Aqueous Solubility Prediction Method
logp	1.413		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3460.00 ± 20.00	kPa	NIST Webbook
pc	3460.00 ± 50.00	kPa	NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	775.30		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	775.30		NIST Webbook

rinpol	748.10		NIST Webbook
rinpol	749.50		NIST Webbook
rinpol	748.10		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	758.00		NIST Webbook
ripol	1121.00		NIST Webbook
ripol	1121.00		NIST Webbook
ripol	1121.00		NIST Webbook
ripol	1167.00		NIST Webbook
tb	427.98	K	Joback Method
tc	576.00 ± 0.70	K	NIST Webbook
tc	576.00 ± 0.50	K	NIST Webbook
tf	188.20	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.81	J/mol×K	427.98	Joback Method
cpg	217.90	J/mol×K	456.00	Joback Method
cpg	227.60	J/mol×K	484.02	Joback Method
cpg	236.93	J/mol×K	512.04	Joback Method
cpg	245.89	J/mol×K	540.06	Joback Method
cpg	254.50	J/mol×K	568.09	Joback Method
cpg	262.76	J/mol×K	596.11	Joback Method
dvisc	0.0095238	Pa×s	268.13	Joback Method
dvisc	0.0545090	Pa×s	228.16	Joback Method
dvisc	0.6544822	Pa×s	188.20	Joback Method
dvisc	0.0026164	Pa×s	308.09	Joback Method
dvisc	0.0009671	Pa×s	348.05	Joback Method
dvisc	0.0004388	Pa×s	388.02	Joback Method
dvisc	0.0002307	Pa×s	427.98	Joback Method
hvapt	52.20	kJ/mol	354.00	NIST Webbook
hvapt	45.40	kJ/mol	371.00	NIST Webbook
hvapt	52.00	kJ/mol	349.50	NIST Webbook
hvapt	44.40	kJ/mol	348.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46925e+01
Coeff. B	-3.04560e+03
Coeff. C	-9.56820e+01
Temperature range (K), min.	307.11
Temperature range (K), max.	420.34

Sources

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

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C565673&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

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

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume