1-Pentanol, 3-methyl-

Other names:	2-Ethyl-4-butanol
	3-Ethyl-1-butanol
	3-Methyl-1-pentanol
	3-Methylpentan-1-ol
	3-Methylpentanol
	3-methylpentyl alcohol
Inchi:	InChI=1S/C6H14O/c1-3-6(2)4-5-7/h6-7H,3-5H2,1-2H3
InchiKey:	IWTBVKIGCDZRPL-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CCC(C)CCO
Mol. weight [g/mol]:	102.17
CAS:	589-35-5

Physical Properties

Property code	Value	Unit	Source
gf	-139.62	kJ/mol	Joback Method
hf	-324.68	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	61.70 ± 0.30	kJ/mol	NIST Webbook
log10ws	-1.36		Crippen Method
logp	1.415		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	852.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	854.50		NIST Webbook
rinpol	829.00		NIST Webbook

rinpol	850.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	807.00		NIST Webbook
rinpol	855.20		NIST Webbook
rinpol	854.40		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	858.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1314.00		NIST Webbook
ripol	1313.00		NIST Webbook
ripol	1341.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1318.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1314.00		NIST Webbook
ripol	1338.00		NIST Webbook
ripol	1297.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1341.00		NIST Webbook
ripol	1320.00		NIST Webbook
ripol	1343.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1343.00		NIST Webbook
ripol	1329.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1344.00		NIST Webbook
ripol	1344.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1309.00		NIST Webbook
tb	424.70	K	NIST Webbook

tb	424.50 ± 0.50	K	NIST Webbook
tb	425.65 ± 2.00	K	NIST Webbook
tb	425.65 ± 3.00	K	NIST Webbook
tb	426.15 ± 2.00	K	NIST Webbook
tb	427.05 ± 0.50	K	NIST Webbook
tb	404.50 ± 0.50	K	NIST Webbook
tb	424.65 ± 2.00	K	NIST Webbook
tb	425.65 ± 3.00	K	NIST Webbook
tb	425.59 ± 0.20	K	NIST Webbook
tb	428.15 ± 2.00	K	NIST Webbook
tb	425.55 ± 1.00	K	NIST Webbook
tb	424.75 ± 2.00	K	NIST Webbook
tb	425.15 ± 2.00	K	NIST Webbook
tb	426.15 ± 1.00	K	NIST Webbook
tc	592.97	K	Joback Method
tf	203.20	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.18	J/mol×K	565.55	Joback Method
cpg	236.05	J/mol×K	510.70	Joback Method
cpg	226.97	J/mol×K	483.27	Joback Method
cpg	217.54	J/mol×K	455.85	Joback Method
cpg	207.74	J/mol×K	428.42	Joback Method
cpg	244.78	J/mol×K	538.12	Joback Method
cpg	261.25	J/mol×K	592.97	Joback Method
dvisc	0.2179366	Pa×s	203.20	Joback Method
dvisc	0.0002400	Pa×s	428.42	Joback Method
dvisc	0.0004330	Pa×s	390.88	Joback Method
dvisc	0.0008856	Pa×s	353.35	Joback Method
dvisc	0.0021472	Pa×s	315.81	Joback Method
dvisc	0.0066108	Pa×s	278.27	Joback Method
dvisc	0.0289027	Pa×s	240.74	Joback Method
hvapt	47.20	kJ/mol	360.50	NIST Webbook
hvapt	54.80	kJ/mol	377.50	NIST Webbook
hvapt	59.70	kJ/mol	362.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45819e+01
Coeff. B	-3.18931e+03
Coeff. C	-1.05903e+02
Temperature range (K), min.	329.02
Temperature range (K), max.	449.93

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
Benchmarks for the fifth industrial fluid properties simulation challenge:	https://www.doi.org/10.1016/j.fluid.2009.07.004
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=C589355&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
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