2-Pentanol, 3-methyl-

Other names:	3-Methyl-2-pentanol
	3-Methyl-4-pentanol
	3-Methylpentan-2-ol
Inchi:	InChI=1S/C6H14O/c1-4-5(2)6(3)7/h5-7H,4H2,1-3H3
InchiKey:	ZXNBBWHRUSXUFZ-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CCC(C)C(C)O
Mol. weight [g/mol]:	102.17
CAS:	565-60-6

Physical Properties

Property code	Value	Unit	Source
gf	-142.06	kJ/mol	Joback Method
hf	-329.96	kJ/mol	Joback Method
hfus	8.34	kJ/mol	Joback Method
hvap	58.20 ± 0.30	kJ/mol	NIST Webbook
log10ws	-0.72		Aqueous Solubility Prediction Method
logp	1.413		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	780.80		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	754.00		NIST Webbook
rinpol	780.00		NIST Webbook
ripol	1212.00		NIST Webbook
ripol	1160.00		NIST Webbook
ripol	1214.00		NIST Webbook

ripol	1160.00		NIST Webbook
ripol	1160.00		NIST Webbook
ripol	1202.00		NIST Webbook
tb	405.70	K	NIST Webbook
tb	407.15 ± 2.00	K	NIST Webbook
tb	407.15 ± 2.00	K	NIST Webbook
tb	406.15 ± 2.00	K	NIST Webbook
tb	405.15 ± 3.00	K	NIST Webbook
tb	407.15 ± 1.00	K	NIST Webbook
tb	407.47 ± 0.20	K	NIST Webbook
tb	407.15 ± 2.00	K	NIST Webbook
tc	596.11	K	Joback Method
tf	188.20	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.50	J/mol×K	568.09	Joback Method
cpg	245.89	J/mol×K	540.06	Joback Method
cpg	236.93	J/mol×K	512.04	Joback Method
cpg	227.60	J/mol×K	484.02	Joback Method
cpg	217.90	J/mol×K	456.00	Joback Method
cpg	207.81	J/mol×K	427.98	Joback Method
cpg	262.76	J/mol×K	596.11	Joback Method
cpl	275.89	J/mol×K	298.15	NIST Webbook
dvisc	0.6544822	Pa×s	188.20	Joback Method
dvisc	0.0002307	Pa×s	427.98	Joback Method
dvisc	0.0004388	Pa×s	388.02	Joback Method
dvisc	0.0009671	Pa×s	348.05	Joback Method
dvisc	0.0026164	Pa×s	308.09	Joback Method
dvisc	0.0095238	Pa×s	268.13	Joback Method
dvisc	0.0545090	Pa×s	228.16	Joback Method
hvapt	60.40	kJ/mol	275.00	NIST Webbook
hvapt	54.40	kJ/mol	361.50	NIST Webbook
hvapt	54.80	kJ/mol	352.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45458e+01
Coeff. B	-3.04350e+03
Coeff. C	-1.00427e+02
Temperature range (K), min.	313.88
Temperature range (K), max.	430.01

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=C565606&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

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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