2-Pentanol, 2,4-dimethyl-

Other names:	2,4-Dimethyl-2-pentanol
	2,4-dimethylpentan-2-ol
	Isobutyldimethylcarbinol
Inchi:	InChI=1S/C7H16O/c1-6(2)5-7(3,4)8/h6,8H,5H2,1-4H3
InchiKey:	FMLSQAUAAGVTJO-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CC(C)CC(C)(C)O
Mol. weight [g/mol]:	116.20
CAS:	625-06-9

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	-0.92		Aqueous Solubility Prediction Method
log10ws	-0.92		Estimated Solubility Method
logp	1.803		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
rinpol	776.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	776.00		NIST Webbook
ripol	1147.00		NIST Webbook
tb	448.07	K	Joback Method
tc	621.71	K	Joback Method
tf	216.89	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	313.99	J/mol×K	621.71	Joback Method
cpg	304.69	J/mol×K	592.77	Joback Method
cpg	294.91	J/mol×K	563.83	Joback Method
cpg	284.62	J/mol×K	534.89	Joback Method
cpg	273.81	J/mol×K	505.95	Joback Method
cpg	262.44	J/mol×K	477.01	Joback Method
cpg	250.49	J/mol×K	448.07	Joback Method
dvisc	0.2459675	Pa×s	216.89	Joback Method
dvisc	0.0002114	Pa×s	448.07	Joback Method
dvisc	0.0003942	Pa×s	409.54	Joback Method
dvisc	0.0008366	Pa×s	371.01	Joback Method
dvisc	0.0021138	Pa×s	332.48	Joback Method
dvisc	0.0068100	Pa×s	293.95	Joback Method
dvisc	0.0312263	Pa×s	255.42	Joback Method
hvapt	49.70	kJ/mol	368.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53993e+01
Coeff. B	-3.53077e+03
Coeff. C	-7.75000e+01
Temperature range (K), min.	311.14
Temperature range (K), max.	427.50

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

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

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=C625069&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