1-Pentanol, 2,2-dimethyl-

Other names:	2,2-Dimethyl-1-pentanol
	2,2-Dimethylpentanol
	2,2-dimethylpentan-1-ol
	Neoheptanol
Inchi:	InChI=1S/C7H16O/c1-4-5-7(2,3)6-8/h8H,4-6H2,1-3H3
InchiKey:	QTOMCRXZFDHJOL-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCC(C)(C)CO
Mol. weight [g/mol]:	116.20
CAS:	2370-12-9

Physical Properties

Property code	Value	Unit	Source
gf	-125.92	kJ/mol	Joback Method
hf	-348.79	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	46.56	kJ/mol	Joback Method
log10ws	-0.82		Aqueous Solubility Prediction Method
log10ws	-1.52		Estimated Solubility Method
logp	1.805		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
rinpol	874.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	874.00		NIST Webbook
ripol	1405.00		NIST Webbook
ripol	1405.00		NIST Webbook
ripol	1405.00		NIST Webbook
tb	425.90 ± 2.00	K	NIST Webbook
tb	427.15 ± 2.00	K	NIST Webbook
tc	618.48	K	Joback Method
tf	231.89	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.39	J/mol×K	448.51	Joback Method
cpg	262.01	J/mol×K	476.84	Joback Method
cpg	273.08	J/mol×K	505.17	Joback Method
cpg	283.62	J/mol×K	533.50	Joback Method
cpg	293.67	J/mol×K	561.82	Joback Method
cpg	303.23	J/mol×K	590.15	Joback Method
cpg	312.34	J/mol×K	618.48	Joback Method
dvisc	0.0985996	Pa×s	231.89	Joback Method
dvisc	0.0179763	Pa×s	267.99	Joback Method
dvisc	0.0049095	Pa×s	304.10	Joback Method
dvisc	0.0017661	Pa×s	340.20	Joback Method
dvisc	0.0007730	Pa×s	376.30	Joback Method
dvisc	0.0003910	Pa×s	412.41	Joback Method
dvisc	0.0002207	Pa×s	448.51	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.70188e+01
Coeff. B	-5.29501e+03
Coeff. C	-1.50000e-01
Temperature range (K), min.	316.62
Temperature range (K), max.	452.43

Sources

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=C2370129&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
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
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