3-Pentanol, 2,3,4-trimethyl-

Other names:	1,1-Diisopropylethanol
	2,3,4-Trimethyl-3-pentanol
Inchi:	InChI=1S/C8H18O/c1-6(2)8(5,9)7(3)4/h6-7,9H,1-5H3
InchiKey:	PLSMHHUFDLYURK-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CC(C)C(C)(O)C(C)C
Mol. weight [g/mol]:	130.23
CAS:	3054-92-0

Physical Properties

Property code	Value	Unit	Source
gf	-122.38	kJ/mol	Joback Method
hf	-379.99	kJ/mol	Joback Method
hfus	6.10	kJ/mol	Joback Method
hvap	48.01	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.049		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
tb	429.65 ± 3.00	K	NIST Webbook
tb	429.65 ± 3.00	K	NIST Webbook
tc	646.51	K	Joback Method
tf	213.16	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.13	J/mol×K	470.51	Joback Method
cpg	306.34	J/mol×K	499.84	Joback Method
cpg	318.90	J/mol×K	529.18	Joback Method
cpg	330.85	J/mol×K	558.51	Joback Method
cpg	342.21	J/mol×K	587.85	Joback Method
cpg	353.00	J/mol×K	617.18	Joback Method

cpg	363.24	J/mol×K	646.51	Joback Method
dvisc	0.4662578	Pa×s	213.16	Joback Method
dvisc	0.0408132	Pa×s	256.05	Joback Method
dvisc	0.0071866	Pa×s	298.94	Joback Method
dvisc	0.0019567	Pa×s	341.84	Joback Method
dvisc	0.0007121	Pa×s	384.73	Joback Method
dvisc	0.0003174	Pa×s	427.62	Joback Method
dvisc	0.0001639	Pa×s	470.51	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.72975e+01
Coeff. B	-5.63683e+03
Coeff. C	1.49230e+01
Temperature range (K), min.	316.46
Temperature range (K), max.	455.36

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=C3054920&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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