3,4,4-Trimethyl-3-pentanol

Other names:	2,2,3-Trimethyl-3-pentanol
	2,2,3-trimethylpentan-3-ol
	3-Pentanol, 2,2,3-trimethyl-
Inchi:	InChI=1S/C8H18O/c1-6-8(5,9)7(2,3)4/h9H,6H2,1-5H3
InchiKey:	KLIHWYNSISMOMR-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCC(C)(O)C(C)(C)C
Mol. weight [g/mol]:	130.23
CAS:	7294-05-5

Physical Properties

Property code	Value	Unit	Source
gf	-114.66	kJ/mol	Joback Method
hf	-378.18	kJ/mol	Joback Method
hfus	5.74	kJ/mol	Joback Method
hvap	47.49	kJ/mol	Joback Method
log10ws	-1.27		Aqueous Solubility Prediction Method
logp	2.194		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
ripol	1289.00		NIST Webbook
ripol	1264.00		NIST Webbook
ripol	1264.00		NIST Webbook
tb	423.65 ± 3.00	K	NIST Webbook
tb	426.65 ± 3.00	K	NIST Webbook
tc	647.15	K	Joback Method
tf	245.58	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.54	J/mol×K	468.16	Joback Method

cpg	309.17	J/mol×K	497.99	Joback Method
cpg	322.04	J/mol×K	527.82	Joback Method
cpg	334.18	J/mol×K	557.66	Joback Method
cpg	345.63	J/mol×K	587.49	Joback Method
cpg	356.43	J/mol×K	617.32	Joback Method
cpg	366.61	J/mol×K	647.15	Joback Method
dvisc	0.1025795	Pa×s	245.58	Joback Method
dvisc	0.0179252	Pa×s	282.68	Joback Method
dvisc	0.0046951	Pa×s	319.77	Joback Method
dvisc	0.0016247	Pa×s	356.87	Joback Method
dvisc	0.0006866	Pa×s	393.97	Joback Method
dvisc	0.0003365	Pa×s	431.06	Joback Method
dvisc	0.0001847	Pa×s	468.16	Joback Method
hvapt	47.30	kJ/mol	372.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57549e+01
Coeff. B	-4.29960e+03
Coeff. C	-4.05700e+01
Temperature range (K), min.	318.55
Temperature range (K), max.	452.27

Sources

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=C7294055&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

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