Ethanol, pentamethyl-

Other names:	2,3,3-Trimethyl-2-butanol
	2-Butanol, 2,3,3-trimethyl-
Inchi:	InChI=1S/C7H16O/c1-6(2,3)7(4,5)8/h8H,1-5H3
InchiKey:	OKXVARYIKDXAEO-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CC(C)(C)C(C)(C)O
Mol. weight [g/mol]:	116.20
CAS:	594-83-2

Physical Properties

Property code	Value	Unit	Source
gf	-123.08	kJ/mol	Joback Method
hf	-357.54	kJ/mol	Joback Method
hfus	3.15	kJ/mol	Joback Method
hvap	45.26	kJ/mol	Joback Method
log10ws	-0.72		Aqueous Solubility Prediction Method
logp	1.803		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
tb	445.28	K	Joback Method
tc	625.83	K	Joback Method
tf	290.15 ± 1.50	K	NIST Webbook
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.88	J/mol×K	445.28	Joback Method
cpg	265.67	J/mol×K	475.37	Joback Method
cpg	277.72	J/mol×K	505.46	Joback Method
cpg	289.06	J/mol×K	535.55	Joback Method
cpg	299.74	J/mol×K	565.64	Joback Method
cpg	309.79	J/mol×K	595.74	Joback Method

cpg	319.24	J/mol×K	625.83	Joback Method
dvisc	0.1416231	Pa×s	234.31	Joback Method
dvisc	0.0242330	Pa×s	269.47	Joback Method
dvisc	0.0062327	Pa×s	304.63	Joback Method
dvisc	0.0021232	Pa×s	339.79	Joback Method
dvisc	0.0008852	Pa×s	374.96	Joback Method
dvisc	0.0004288	Pa×s	410.12	Joback Method
dvisc	0.0002329	Pa×s	445.28	Joback Method
hvapt	48.70	kJ/mol	330.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.73281e+01
Coeff. B	-4.30672e+03
Coeff. C	-6.41500e+01
Temperature range (K), min.	290.15
Temperature range (K), max.	422.55

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C594832&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume