1-Pentanol, 2-ethyl-

Other names:	2-Ethyl-1-pentanol
	2-ethylpentan-1-ol
Inchi:	InChI=1S/C7H16O/c1-3-5-7(4-2)6-8/h7-8H,3-6H2,1-2H3
InchiKey:	UKFQWAVMIMCNEH-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCC(CC)CO
Mol. weight [g/mol]:	116.20
CAS:	27522-11-8

Physical Properties

Property code	Value	Unit	Source
gf	-131.20	kJ/mol	Joback Method
hf	-345.32	kJ/mol	Joback Method
hfus	14.45	kJ/mol	Joback Method
hvap	47.47	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.805		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	439.15 ± 3.00	K	NIST Webbook
tb	426.65 ± 5.00	K	NIST Webbook
tb	438.15 ± 2.00	K	NIST Webbook
tb	438.15 ± 3.00	K	NIST Webbook
tc	615.06	K	Joback Method
tf	214.47	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.92	J/mol×K	451.30	Joback Method
cpg	258.79	J/mol×K	478.59	Joback Method
cpg	269.25	J/mol×K	505.89	Joback Method
cpg	279.32	J/mol×K	533.18	Joback Method

cpg	289.00	J/mol×K	560.47	Joback Method
cpg	298.30	J/mol×K	587.77	Joback Method
cpg	307.23	J/mol×K	615.06	Joback Method
dvisc	0.1594974	Pa×s	214.47	Joback Method
dvisc	0.0221021	Pa×s	253.94	Joback Method
dvisc	0.0052125	Pa×s	293.41	Joback Method
dvisc	0.0017316	Pa×s	332.88	Joback Method
dvisc	0.0007266	Pa×s	372.36	Joback Method
dvisc	0.0003601	Pa×s	411.83	Joback Method
dvisc	0.0002018	Pa×s	451.30	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.71974e+01
Coeff. B	-5.35202e+03
Coeff. C	-1.36810e+01
Temperature range (K), min.	330.18
Temperature range (K), max.	463.96

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27522118&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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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