1-Pentanol, 2-ethyl-4-methyl-

Other names:	2-Ethyl-4-methylpentanol
	2-Ethylisohexanol
	2-Ethyl-4-methyl-1-pentanol
	2-ethyl-4-methylpentan-1-ol
	2-Methyl-1-heptanol
Inchi:	InChI=1S/C8H18O/c1-4-8(6-9)5-7(2)3/h7-9H,4-6H2,1-3H3
InchiKey:	QCHSJPKDWOFACC-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCC(CO)CC(C)C
Mol. weight [g/mol]:	130.23
CAS:	106-67-2

Physical Properties

Property code	Value	Unit	Source
gf	-125.22	kJ/mol	Joback Method
hf	-371.24	kJ/mol	Joback Method
hfus	13.52	kJ/mol	Joback Method
hvap	49.31	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	2.051		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	962.00		NIST Webbook
rinpol	948.00		NIST Webbook
tb	449.65 ± 3.00	K	NIST Webbook
tc	639.93	K	Joback Method
tf	210.74	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.39	J/mol×K	473.74	Joback Method
cpg	302.54	J/mol×K	501.44	Joback Method

cpg	314.22	J/mol×K	529.14	Joback Method
cpg	325.44	J/mol×K	556.84	Joback Method
cpg	336.21	J/mol×K	584.53	Joback Method
cpg	346.54	J/mol×K	612.23	Joback Method
cpg	356.45	J/mol×K	639.93	Joback Method
dvisc	0.3001577	Pa×s	210.74	Joback Method
dvisc	0.0290327	Pa×s	254.57	Joback Method
dvisc	0.0055777	Pa×s	298.41	Joback Method
dvisc	0.0016351	Pa×s	342.24	Joback Method
dvisc	0.0006333	Pa×s	386.07	Joback Method
dvisc	0.0002977	Pa×s	429.91	Joback Method
dvisc	0.0001609	Pa×s	473.74	Joback Method
hvapt	53.30	kJ/mol	399.50	NIST Webbook

Sources

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=C106672&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume