

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	m ³ /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/molxK	529.14	Joback Method
cpg	325.44	J/molxK	556.84	Joback Method
cpg	336.21	J/molxK	584.53	Joback Method
cpg	346.54	J/molxK	612.23	Joback Method
cpg	356.45	J/molxK	639.93	Joback Method
dvisc	0.3001577	Paxs	210.74	Joback Method
dvisc	0.0290327	Paxs	254.57	Joback Method
dvisc	0.0055777	Paxs	298.41	Joback Method
dvisc	0.0016351	Paxs	342.24	Joback Method
dvisc	0.0006333	Paxs	386.07	Joback Method
dvisc	0.0002977	Paxs	429.91	Joback Method
dvisc	0.0001609	Paxs	473.74	Joback Method
hvapt	53.30	kJ/mol	399.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106672&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

tf: Normal melting (fusion) point

vc: Critical Volume

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