

Pentane, 1-ethoxy-

Other names:	1-ethoxy-pentane Amyl ethyl ether Ether, ethyl pentyl Ethyl amyl ether Ethyl pentyl ether n-C5H11OC2H5
Inchi:	InChI=1S/C7H16O/c1-3-5-6-7-8-4-2/h3-7H2,1-2H3
InchiKey:	VDMXPMYSWFDBJB-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCCCOCC
Mol. weight [g/mol]:	116.20
CAS:	17952-11-3

Physical Properties

Property code	Value	Unit	Source
gf	-96.94	kJ/mol	Joback Method
hf	-320.03	kJ/mol	Joback Method
hfus	15.07	kJ/mol	Joback Method
hvap	41.06	kJ/mol	NIST Webbook
ie	9.49	eV	NIST Webbook
log10ws	-1.84		Crippen Method
logp	2.213		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	742.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	769.50		NIST Webbook
rinpol	774.70		NIST Webbook
tb	392.70	K	NIST Webbook
tb	390.70	K	NIST Webbook
tc	546.34	K	Joback Method
tf	190.88	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.30	J/mol×K	546.34	Joback Method
cpg	218.44	J/mol×K	381.98	Joback Method
cpg	229.92	J/mol×K	409.37	Joback Method
cpg	241.06	J/mol×K	436.77	Joback Method
cpg	251.87	J/mol×K	464.16	Joback Method
cpg	262.35	J/mol×K	491.56	Joback Method
cpg	272.49	J/mol×K	518.95	Joback Method
dvisc	0.0002231	Pa×s	381.98	Joback Method
dvisc	0.0039006	Pa×s	190.88	Joback Method
dvisc	0.0017217	Pa×s	222.73	Joback Method
dvisc	0.0009325	Pa×s	254.58	Joback Method
dvisc	0.0005789	Pa×s	286.43	Joback Method
dvisc	0.0003953	Pa×s	318.28	Joback Method
dvisc	0.0002894	Pa×s	350.13	Joback Method
hvapt	34.41	kJ/mol	390.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51833e+01
Coeff. B	-3.62296e+03
Coeff. C	-4.97780e+01
Temperature range (K), min.	293.00
Temperature range (K), max.	416.78

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=C17952113&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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