Ether, ethyl 4-methyl-1-pentyl, (E)

Inchi: InChI=1S/C8H16O/c1-4-9-7-5-6-8(2)3/h5,7-8H,4,6H2,1-3H3/b7-5+
InchiKey: PEGWCMWUBAGRKQ-FNORWQNLSA-N
Formula: C8H16O
SMILES: CCOC=CCC(C)C
Mol. weight [g/mol]: 128.21
CAS: 16969-14-5

Physical Properties

Property code	Value	Unit	Source
gf	-10.74	kJ/mol	Joback Method
hf	-228.73	kJ/mol	Joback Method
hfus	14.34	kJ/mol	Joback Method
hvap	35.38	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.583		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
tb	408.58	K	Joback Method
tc	584.62	K	Joback Method
tf	182.07	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.63	J/mol×K	408.58	Joback Method
cpg	302.28	J/mol×K	555.28	Joback Method
cpg	291.29	J/mol×K	525.94	Joback Method
cpg	279.84	J/mol×K	496.60	Joback Method
cpg	267.93	J/mol×K	467.26	Joback Method
cpg	255.52	J/mol×K	437.92	Joback Method
cpg	312.81	J/mol×K	584.62	Joback Method
dvisc	0.0001752	Pa×s	408.58	Joback Method
dvisc	0.0002362	Pa×s	370.83	Joback Method

dvisc	0.0003409	Pa×s	333.08	Joback Method
dvisc	0.0005403	Pa×s	295.32	Joback Method
dvisc	0.0009800	Pa×s	257.57	Joback Method
dvisc	0.0021811	Pa×s	219.82	Joback Method
dvisc	0.0067640	Pa×s	182.07	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16969145&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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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