

4-Methyl-2-pentanol, methyl ether

Inchi:	InChI=1S/C7H16O/c1-6(2)5-7(3)8-4/h6-7H,5H2,1-4H3
InchiKey:	XOQBTEUBXZXNKK-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	COC(C)CC(C)C
Mol. weight [g/mol]:	116.20

Physical Properties

Property code	Value	Unit	Source
gf	-101.82	kJ/mol	Joback Method
hf	-330.59	kJ/mol	Joback Method
hfus	8.03	kJ/mol	Joback Method
hvap	32.81	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	2.067		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	734.60		NIST Webbook
tb	381.10	K	Joback Method
tc	553.18	K	Joback Method
tf	160.88	K	Joback Method
vc	0.433	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.23	J/molxK	381.10	Joback Method
cpg	230.43	J/molxK	409.78	Joback Method
cpg	242.25	J/molxK	438.46	Joback Method
cpg	253.69	J/molxK	467.14	Joback Method
cpg	264.76	J/molxK	495.82	Joback Method
cpg	275.45	J/molxK	524.50	Joback Method
cpg	285.76	J/molxK	553.18	Joback Method
dvisc	0.0138704	Paxs	160.88	Joback Method
dvisc	0.0036036	Paxs	197.58	Joback Method

dvisc	0.0014282	Paxs	234.29	Joback Method
dvisc	0.0007273	Paxs	270.99	Joback Method
dvisc	0.0004351	Paxs	307.69	Joback Method
dvisc	0.0002904	Paxs	344.40	Joback Method
dvisc	0.0002095	Paxs	381.10	Joback Method

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=U333935&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
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

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