

4-Methoxy-4-methyl-1-pentanol

Inchi:	InChI=1S/C7H16O2/c1-7(2,9-3)5-4-6-8/h8H,4-6H2,1-3H3
InchiKey:	BVLZIEGHZCFNSG-UHFFFAOYSA-N
Formula:	C7H16O2
SMILES:	COC(C)(C)CCCO
Mol. weight [g/mol]:	132.20

Physical Properties

Property code	Value	Unit	Source
gf	-230.92	kJ/mol	Joback Method
hf	-481.01	kJ/mol	Joback Method
hfus	11.75	kJ/mol	Joback Method
hvap	48.97	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.184		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	911.00		NIST Webbook
rinpol	895.00		NIST Webbook
tb	470.93	K	Joback Method
tc	640.66	K	Joback Method
tf	254.12	K	Joback Method
vc	0.454	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.26	J/molxK	470.93	Joback Method
cpg	326.25	J/molxK	612.37	Joback Method
cpg	316.76	J/molxK	584.08	Joback Method
cpg	306.83	J/molxK	555.80	Joback Method
cpg	296.44	J/molxK	527.51	Joback Method
cpg	285.59	J/molxK	499.22	Joback Method
cpg	335.31	J/molxK	640.66	Joback Method
dvisc	0.0001621	Paxs	470.93	Joback Method

dvisc	0.0002778	Paxs	434.79	Joback Method
dvisc	0.0005248	Paxs	398.66	Joback Method
dvisc	0.0011255	Paxs	362.52	Joback Method
dvisc	0.0028582	Paxs	326.39	Joback Method
dvisc	0.0091543	Paxs	290.25	Joback Method
dvisc	0.0408253	Paxs	254.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R142675&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

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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