4-Methoxy-4-methyl-2-pentanol

Other names: 2-Pentanol, 4-methoxy-4-methyl-
4-Methyl-4-methoxy-2-pentanol
Inchi: InChI=1S/C7H16O2/c1-6(8)5-7(2,3)9-4/h6,8H,5H2,1-4H3
InchiKey: OMSLSFZIEVFEIH-UHFFFAOYSA-N
Formula: C7H16O2
SMILES: COC(C)(C)CC(C)O
Mol. weight [g/mol]: 132.20
CAS: 141-73-1

Physical Properties

Property code	Value	Unit	Source
gf	-233.36	kJ/mol	Joback Method
hf	-486.29	kJ/mol	Joback Method
hfus	8.22	kJ/mol	Joback Method
hvap	48.58	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.182		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
tb	470.49	K	Joback Method
tc	643.77	K	Joback Method
tf	239.12	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.42	J/mol×K	470.49	Joback Method
cpg	286.06	J/mol×K	499.37	Joback Method
cpg	297.20	J/mol×K	528.25	Joback Method
cpg	307.84	J/mol×K	557.13	Joback Method
cpg	318.00	J/mol×K	586.01	Joback Method
cpg	327.70	J/mol×K	614.89	Joback Method
cpg	336.95	J/mol×K	643.77	Joback Method

dvisc	0.0888370	Pa×s	239.12	Joback Method
dvisc	0.0147686	Pa×s	277.68	Joback Method
dvisc	0.0038030	Pa×s	316.24	Joback Method
dvisc	0.0013152	Pa×s	354.81	Joback Method
dvisc	0.0005601	Pa×s	393.37	Joback Method
dvisc	0.0002778	Pa×s	431.93	Joback Method
dvisc	0.0001546	Pa×s	470.49	Joback Method
hvapt	46.60	kJ/mol	383.00	NIST Webbook

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=C141731&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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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