

Pentane, 2-methoxy-2-methyl-

Inchi:	InChI=1S/C7H16O/c1-5-6-7(2,3)8-4/h5-6H2,1-4H3
InchiKey:	WYLQOLGJMFRLX-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCC(C)(C)OC
Mol. weight [g/mol]:	116.20

Physical Properties

Property code	Value	Unit	Source
gf	-94.10	kJ/mol	Joback Method
hf	-328.78	kJ/mol	Joback Method
hfus	7.66	kJ/mol	Joback Method
hvap	32.29	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	2.212		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
rinpola	763.00		NIST Webbook
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tb	378.75	K	Joback Method
tc	553.95	K	Joback Method
tf	193.30	K	Joback Method
vc	0.434	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.51	J/molxK	378.75	Joback Method
cpg	232.48	J/molxK	407.95	Joback Method
cpg	244.93	J/molxK	437.15	Joback Method
cpg	256.86	J/molxK	466.35	Joback Method
cpg	268.29	J/molxK	495.55	Joback Method
cpg	279.24	J/molxK	524.75	Joback Method
cpg	289.71	J/molxK	553.95	Joback Method
dvisc	0.0073885	Paxs	193.30	Joback Method

dvisc	0.0028572	Paxs	224.21	Joback Method
dvisc	0.0013910	Paxs	255.12	Joback Method
dvisc	0.0007911	Paxs	286.02	Joback Method
dvisc	0.0005023	Paxs	316.93	Joback Method
dvisc	0.0003458	Paxs	347.84	Joback Method
dvisc	0.0002529	Paxs	378.75	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R73036&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
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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