pentane, 2-methoxy-2-methyl-

Inchi: InChI=1S/C7H16O/c1-5-6-7(2,3)8-4/h5-6H2,1-4H3
InchiKey: WYLQOLGJMFRRLX-UHFFFAOYSA-N
Formula: C7H16O
SMILES: CCCC(C)(C)OC
Mol. weight [g/mol]: 116.20
CAS: 38772-53-1

Physical Properties

Property code	Value	Unit	Source
af	0.3266		Cheméo Relay (1.0)
gf	-94.10	kJ/mol	Joback Method
hf	-325.13	kJ/mol	Cheméo Relay (1.0)
hfus	7.66	kJ/mol	Joback Method
hvap	37.46	kJ/mol	Cheméo Relay (1.0)
log10ws	-1.22		Cheméo Relay (1.0)
logp	2.212		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
tb	376.79	K	Cheméo Relay (1.0)
tc	548.43	K	Cheméo Relay (1.0)
tf	157.30	K	Cheméo Relay (1.0)
vc	0.419	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

dvisc	0.0028572	Pa×s	224.21	Joback Method
dvisc	0.0013910	Pa×s	255.12	Joback Method
dvisc	0.0007911	Pa×s	286.02	Joback Method
dvisc	0.0005023	Pa×s	316.93	Joback Method
dvisc	0.0003458	Pa×s	347.84	Joback Method
dvisc	0.0002529	Pa×s	378.75	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38772531&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.