Pentane, 1,1-dimethoxy

Other names: 1,1-dimethoxypentane
Inchi: InChI=1S/C7H16O2/c1-4-5-6-7(8-2)9-3/h7H,4-6H2,1-3H3
InchiKey: VMOZJXZMOQSSMH-UHFFFAOYSA-N
Formula: C7H16O2
SMILES: CCCCC(OC)OC
Mol. weight [g/mol]: 132.20
CAS: 26450-58-8

Physical Properties

Property code	Value	Unit	Source
gf	-204.38	kJ/mol	Joback Method
hf	-457.53	kJ/mol	Joback Method
hfus	12.74	kJ/mol	Joback Method
hvap	35.61	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.796		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	868.00		NIST Webbook
rinpol	868.00		NIST Webbook
ripol	1057.00		NIST Webbook
tb	403.96	K	Joback Method
tc	572.52	K	Joback Method
tf	198.11	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.30	J/mol×K	403.96	Joback Method
cpg	297.29	J/mol×K	544.43	Joback Method
cpg	286.90	J/mol×K	516.33	Joback Method
cpg	276.21	J/mol×K	488.24	Joback Method
cpg	265.20	J/mol×K	460.15	Joback Method

cpg	253.90	J/mol×K	432.05	Joback Method
cpg	307.36	J/mol×K	572.52	Joback Method
dvisc	0.0001919	Pa×s	403.96	Joback Method
dvisc	0.0002559	Pa×s	369.65	Joback Method
dvisc	0.0003618	Pa×s	335.34	Joback Method
dvisc	0.0005536	Pa×s	301.04	Joback Method
dvisc	0.0009450	Pa×s	266.73	Joback Method
dvisc	0.0018890	Pa×s	232.42	Joback Method
dvisc	0.0047999	Pa×s	198.11	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C26450588&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from: