4-Methyl-2-pentanone dimethylacetal

Inchi: InChI=1S/C8H18O2/c1-7(2)6-8(3,9-4)10-5/h7H,6H2,1-5H3
InchiKey: WCPUFSIDCWSGEW-UHFFFAOYSA-N
Formula: C8H18O2
SMILES: COC(C)(CC(C)C)OC
Mol. weight [g/mol]: 146.23
CAS: 1112-78-3

Physical Properties

Property code	Value	Unit	Source
gf	-193.12	kJ/mol	Joback Method
hf	-486.92	kJ/mol	Joback Method
hfus	7.92	kJ/mol	Joback Method
hvap	36.54	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	2.042		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
tb	423.61	K	Joback Method
tc	602.03	K	Joback Method
tf	211.80	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.39	J/mol×K	423.61	Joback Method
cpg	349.90	J/mol×K	572.29	Joback Method
cpg	337.84	J/mol×K	542.55	Joback Method
cpg	325.27	J/mol×K	512.82	Joback Method
cpg	312.17	J/mol×K	483.08	Joback Method
cpg	298.55	J/mol×K	453.35	Joback Method
cpg	361.46	J/mol×K	602.03	Joback Method
dvisc	0.0001947	Pa×s	423.61	Joback Method
dvisc	0.0002736	Pa×s	388.31	Joback Method

dvisc	0.0004117	Pa×s	353.01	Joback Method
dvisc	0.0006783	Pa×s	317.71	Joback Method
dvisc	0.0012661	Pa×s	282.40	Joback Method
dvisc	0.0028247	Pa×s	247.10	Joback Method
dvisc	0.0082347	Pa×s	211.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1112783&Units=SI
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

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