2-Pentanone, 5,5-diethoxy-

Other names: Levulinaldehyde, 1-(diethyl acetal)
1,1-Diethoxypentan-4-one
5,5-Diethoxypentan-2-one
Inchi: InChI=1S/C9H18O3/c1-4-11-9(12-5-2)7-6-8(3)10/h9H,4-7H2,1-3H3
InchiKey: BRQZMIVIOUPIFN-UHFFFAOYSA-N
Formula: C9H18O3
SMILES: CCOC(CCC(C)=O)OCC
Mol. weight [g/mol]: 174.24
CAS: 14499-41-3

Physical Properties

Property code	Value	Unit	Source
gf	-316.46	kJ/mol	Joback Method
hf	-611.39	kJ/mol	Joback Method
hfus	19.52	kJ/mol	Joback Method
hvap	46.81	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.755		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1158.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1162.00		NIST Webbook
ripol	1563.00		NIST Webbook
tb	503.59	K	Joback Method
tc	680.25	K	Joback Method
tf	270.58	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	348.25	J/mol×K	503.59	Joback Method
cpg	410.59	J/mol×K	650.81	Joback Method
cpg	399.06	J/mol×K	621.36	Joback Method
cpg	387.05	J/mol×K	591.92	Joback Method
cpg	374.58	J/mol×K	562.48	Joback Method
cpg	361.64	J/mol×K	533.03	Joback Method
cpg	421.65	J/mol×K	680.25	Joback Method
dvisc	0.0001875	Pa×s	503.59	Joback Method
dvisc	0.0002481	Pa×s	464.75	Joback Method
dvisc	0.0003454	Pa×s	425.92	Joback Method
dvisc	0.0005138	Pa×s	387.09	Joback Method
dvisc	0.0008351	Pa×s	348.25	Joback Method
dvisc	0.0015333	Pa×s	309.41	Joback Method
dvisc	0.0033518	Pa×s	270.58	Joback Method

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=C14499413&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
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