Ethanone, 1-(3-methyloxiranyl)-

Other names: 2-Pentanone, 3,4-epoxy-
3,4-Epoxy-2-pentanone
Inchi: InChI=1S/C5H8O2/c1-3(6)5-4(2)7-5/h4-5H,1-2H3
InchiKey: IAHUKWSQLBRAIN-UHFFFAOYSA-N
Formula: C5H8O2
SMILES: CC(=O)C1OC1C
Mol. weight [g/mol]: 100.12
CAS: 17257-79-3

Physical Properties

Property code	Value	Unit	Source
gf	-170.78	kJ/mol	Joback Method
hf	-338.65	kJ/mol	Joback Method
hfus	17.49	kJ/mol	Joback Method
hvap	37.58	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	0.363		Crippen Method
mcvol	77.890	ml/mol	McGowan Method
pc	4178.49	kPa	Joback Method
ripol	1263.00		NIST Webbook
ripol	1263.00		NIST Webbook
tb	396.69	K	Joback Method
tc	591.36	K	Joback Method
tf	236.31	K	Joback Method
vc	0.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.21	J/mol×K	396.69	Joback Method
cpg	162.27	J/mol×K	429.14	Joback Method
cpg	171.81	J/mol×K	461.58	Joback Method
cpg	180.84	J/mol×K	494.03	Joback Method
cpg	189.39	J/mol×K	526.47	Joback Method

cpg	197.47	J/mol×K	558.92	Joback Method
cpg	205.12	J/mol×K	591.36	Joback Method
dvisc	0.0011617	Pa×s	236.31	Joback Method
dvisc	0.0009407	Pa×s	263.04	Joback Method
dvisc	0.0007920	Pa×s	289.77	Joback Method
dvisc	0.0006864	Pa×s	316.50	Joback Method
dvisc	0.0006083	Pa×s	343.23	Joback Method
dvisc	0.0005486	Pa×s	369.96	Joback Method
dvisc	0.0005017	Pa×s	396.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17257793&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume