2,3-Butanedione, mono(O-methyloxime)

Other names:	1-Acetyl-1-methoxyiminoethane
	2,3-Butanedione-2-methoxime
Inchi:	InChI=1S/C5H9NO2/c1-4(5(2)7)6-8-3/h1-3H3
InchiKey:	LBTXDQOSJLEDQM-UHFFFAOYSA-N
Formula:	C5H9NO2
SMILES:	CON=C(C)C(C)=O
Mol. weight [g/mol]:	115.13
CAS:	617-32-3

Physical Properties

Property code	Value	Unit	Source
hf	-318.90	kJ/mol	Joback Method
hvap	39.27	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	0.598		Crippen Method
mcvol	94.430	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
tb	466.65	K	Joback Method
tc	670.90	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C617323&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

hf:	Enthalpy of formation 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