2,3-Butanedione-2-methoxime

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

Physical Properties

Property code	Value	Unit	Source
ie	9.31	eV	Cheméo Relay (1.0)
logp	0.598		Crippen Method
mcvol	94.430	ml/mol	McGowan Method
tb	415.07	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C617323&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature