

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.cheméo.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

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