Butanal, O-methyloxime

Inchi: InChI=1S/C5H11NO/c1-3-4-5-6-7-2/h5H,3-4H2,1-2H3
InchiKey: BMDFNHAUSSAITP-UHFFFAOYSA-N
Formula: C5H11NO
SMILES: CCCC=NOC
Mol. weight [g/mol]: 101.15
CAS: 31376-98-4

Physical Properties

Property code	Value	Unit	Source
hf	-196.53	kJ/mol	Joback Method
hvap	32.45	kJ/mol	Joback Method
ie	9.33 ± 0.05	eV	NIST Webbook
log10ws	-1.16		Crippen Method
logp	1.419		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	680.00		NIST Webbook
rinpol	680.00		NIST Webbook
tb	412.90	K	Joback Method
tc	601.66	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C31376984&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature