ISOVALERALDEHYDE OXIME

Other names:	3-Methylbutanal oxime
	3-methylbutyraldehyde oxime
	3)Methyl-butyl-aldoxime
Inchi:	InChI=1S/C5H11NO/c1-5(2)3-4-6-7/h4-5,7H,3H2,1-2H3
InchiKey:	JAUPRNSQRRCCRR-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CC(C)CC=NO
Mol. weight [g/mol]:	101.15

Physical Properties

Property code	Value	Unit	Source
hvap	52.42	kJ/mol	Cheméo Relay (1.0)
ie	9.55	eV	Cheméo Relay (1.0)
logp	1.492		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
rinpol	858.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	858.00		NIST Webbook
tb	416.22	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C626904&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

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature