Methyl nitrite

Other names:	Nitrous acid, methyl ester
	CH3ONO
	Methylester kyseliny dusite
	Methyl ester of nitrous acid
Inchi:	InChI=1S/CH3NO2/c1-4-2-3/h1H3
InchiKey:	BLLFVUPNHCTMSV-UHFFFAOYSA-N
Formula:	CH3NO2
SMILES:	CON=O
Mol. weight [g/mol]:	61.04
CAS:	624-91-9

Physical Properties

Property code	Value	Unit	Source
affp	798.90	kJ/mol	NIST Webbook
basg	766.40	kJ/mol	NIST Webbook
chg	-752.00 ± 3.00	kJ/mol	NIST Webbook
hf	-65.44 ± 0.84	kJ/mol	NIST Webbook
hf	-62.50 ± 1.10	kJ/mol	NIST Webbook
hf	-70.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-67.15 ± 0.84	kJ/mol	NIST Webbook
hfl	-85.10 ± 1.00	kJ/mol	NIST Webbook
hvap	22.60 ± 0.20	kJ/mol	NIST Webbook
ie	11.00	eV	NIST Webbook
ie	10.47 ± 0.01	eV	NIST Webbook
ie	10.44	eV	NIST Webbook
ie	10.38 ± 0.03	eV	NIST Webbook
ie	10.30	eV	NIST Webbook
ie	10.38 ± 0.03	eV	NIST Webbook
ie	10.38	eV	NIST Webbook
log10ws	-0.51		Crippen Method
logp	0.314		Crippen Method
mcvol	42.370	ml/mol	McGowan Method
pc	5495.11	kPa	Joback Method
rinpol	268.00		NIST Webbook
tb	308.10	K	Joback Method
tc	476.03	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	22.10	kJ/mol	245.50	NIST Webbook
hvapt	26.20	kJ/mol	189.50	NIST Webbook

Sources

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=C624919&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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