2-Propanone, oxime

Other names:	Acetone, oxime
	«beta»-Isonitrosopropane
	Acetoxime
	(CH3)2C=NOH
	Acetonoxime
Inchi:	InChI=1S/C3H7NO/c1-3(2)4-5/h5H,1-2H3
InchiKey:	PXAJQJMDEXJWFB-UHFFFAOYSA-N
Formula:	C3H7NO
SMILES:	CC(C)=NO
Mol. weight [g/mol]:	73.09
CAS:	127-06-0

Physical Properties

Property code	Value	Unit	Source
chs	-2052.00	kJ/mol	NIST Webbook
hf	-185.05	kJ/mol	Joback Method
hfs	-140.00	kJ/mol	NIST Webbook
hvap	42.34	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
ie	9.67	eV	NIST Webbook
log10ws	0.10		Crippen Method
logp	0.856		Crippen Method
mcvol	64.680	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
rinpol	700.00		NIST Webbook
tb	406.00	K	NIST Webbook
tb	408.20	K	NIST Webbook
tc	624.72	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	59.60	kJ/mol	323.00	NIST Webbook
hvapt	51.40	kJ/mol	345.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C127060&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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

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