ACETONE THIOSEMICARBAZONE

Other names:	Acetone, thiosemicarbazone
	Thiosemicarbazone acetone
	Acetonthiosemikarbazon
	2-(1-Methylethylidene)hydrazinecarbothioamide
Inchi:	InChI=1S/C4H9N3S/c1-3(2)6-7-4(5)8/h1-2H3,(H3,5,7,8)
InchiKey:	FQUDPIIGGVBZEQ-UHFFFAOYSA-N
Formula:	C4H9N3S
SMILES:	CC(C)=NNC(N)=S
Mol. weight [g/mol]:	131.20

Physical Properties

Property code	Value	Unit	Source
chs	-3483.00	kJ/mol	NIST Webbook
hfs	21.00 ± 3.00	kJ/mol	NIST Webbook
ie	7.70	eV	Cheméo Relay (1.0)
logp	0.215		Crippen Method
mcvol	104.910	ml/mol	McGowan Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1752303&Units=SI

Legend

chs:	Standard solid enthalpy of combustion

hfs:	Solid phase enthalpy of formation at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume