2-PYRROLIDINETHIONE, 1-METHYL-

Other names: N-Methyl-2-thiopyrrolidinone
Inchi: InChI=1S/C5H9NS/c1-6-4-2-3-5(6)7/h2-4H2,1H3
InchiKey: OQILOJRSIWGQSM-UHFFFAOYSA-N
Formula: C5H9NS
SMILES: CN1CCCC1=S
Mol. weight [g/mol]: 115.20

Physical Properties

Property code	Value	Unit	Source
hf	38.66	kJ/mol	Cheméo Relay (1.0)
hvap	69.31	kJ/mol	Cheméo Relay (1.0)
ie	7.95	eV	Cheméo Relay (1.0)
log10ws	-0.83		Cheméo Relay (1.0)
logp	1.039		Crippen Method
mcvol	92.480	ml/mol	McGowan Method
pc	4331.12	kPa	Cheméo Relay (1.0, beta)
tb	501.60	K	Cheméo Relay (1.0)
tc	738.66	K	Cheméo Relay (1.0)
tf	280.42	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10441573&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point