Acetone beta-mercaptopropionhydrazone

Inchi: InChI=1S/C6H12N2OS/c1-5(2)7-8-6(9)3-4-10/h10H,3-4H2,1-2H3,(H,8,9)
InchiKey: PFJRVRPQETVUTA-UHFFFAOYSA-N
Formula: C6H12N2OS
SMILES: CC(C)=NNC(=O)CCS
Mol. weight [g/mol]: 160.24
CAS: 689-42-9

Physical Properties

Property code	Value	Unit	Source
hf	-115.37	kJ/mol	Joback Method
hvap	52.26	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	0.818		Crippen Method
mcvol	128.980	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
tb	580.14	K	Joback Method
tc	804.06	K	Joback Method

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=C689429&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
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