2-mercaptoimidazole

Other names:	1,3-dihydro-2H-imidazole-2-thione
	1,3-dihydroimidazole-2-thione
Inchi:	InChI=1S/C3H4N2S/c6-3-4-1-2-5-3/h1-2H,(H2,4,5,6)
InchiKey:	OXFSTTJBVAAALW-UHFFFAOYSA-N
Formula:	C3H4N2S
SMILES:	S=c1[nH]cc[nH]1
Mol. weight [g/mol]:	100.15

Physical Properties

Property code	Value	Unit	Source
hfus	17.48	kJ/mol	Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies
log10ws	-0.76		Crippen Method
logp	0.108		Crippen Method
mcvol	69.980	ml/mol	McGowan Method
tt	503.50	K	Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cps	112.00	J/mol×K	298.15	Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies
cps	112.40	J/mol×K	303.15	Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies
cps	112.90	J/mol×K	308.15	Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies
cps	112.60	J/mol×K	313.15	Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies
cps	113.40	J/mol×K	318.15	Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies

cps	114.30	J/mol×K	323.15	Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies
cps	115.30	J/mol×K	328.15	Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies
cps	116.50	J/mol×K	333.15	Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies
hvapt	114.40	kJ/mol	298.15	Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies
rhos	1424.10	kg/m3	296.00	Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies

Sources

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
Structural and energetic characterization of anhydrous and hemihydrated 2-mercaptoimidazole: Calorimetric, X-ray diffraction, and computational studies:	https://www.doi.org/10.1016/j.jct.2015.11.010

Legend

cps:	Solid phase heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rhos:	Solid Density
tt:	Triple Point Temperature