

Isatin, 3-thiosemicarbazone

Other names:	(1,2-dihydro-2-oxo-3H-indol-3-yl) thiosemicarbazone
Inchi:	InChI=1S/C9H8N4OS/c10-9(15)13-12-7-5-3-1-2-4-6(5)11-8(7)14/h1-4H,(H3,10,13,15)(H,
InchiKey:	SLEMRAMJSGBARH-UHFFFAOYSA-N
Formula:	C9H8N4OS
SMILES:	NC(=S)NN=C1C(=O)Nc2ccccc21
Mol. weight [g/mol]:	220.25
CAS:	487-16-1

Physical Properties

Property code	Value	Unit	Source
hf	264.01	kJ/mol	Joback Method
hvap	77.74	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	0.176		Crippen Method
mcvol	152.290	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
tb	836.66	K	Joback Method
tc	1118.68	K	Joback Method

Sources

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=C487161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.cheméo.com/cid/69-604-5/Isatin-3-thiosemicarbazone.pdf>

Generated by Cheméo on 2025-12-05 10:15:04.226934446 +0000 UTC m=+4677901.756975110.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.