

1-(N,n-dimethylthiocarbamoylthio)-2-propanone

2,4-dinitrophenyl-hydrazone
InChI=1S/C12H15N5O4S2/c1-8/7-23-12(22)15(2)3)13-14-10-5-4-9(16(18)19)6-11(10)17
InChIKey: ISVXACVOHBRKMK-UHFFFAOYSA-N

Formula: C12H15N5O4S2
SMILES: CC(CSC(=S)N(C)C)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 357.41
CAS: 96432-96-1

Physical Properties

Property code	Value	Unit	Source
hf	282.86	kJ/mol	Joback Method
hvap	104.51	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	2.870		Crippen Method
mcvol	245.060	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
tb	1092.27	K	Joback Method
tc	1373.74	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=C96432961&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

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