

# N-Isopropyl-N'-methyl-N,N'-bis(trifluoroacetyl)-6-methylthio-1,3,5-triazine-2,4-diamine

**Other names:** 1,3,5-Triazine-2,4-diamine,  
**Inchi:** N-methyl-N'-(1-methylethyl)-N,N'-bis-trifluoroacetyl-6-(methylthio)-1,3,5-triazine-2,4-diamine  
**InchiKey:** LSHSXPWJOJLWCD-UHFFFAOYSA-N  
**Formula:** C<sub>12</sub>H<sub>13</sub>F<sub>6</sub>N<sub>5</sub>O<sub>2</sub>S  
**SMILES:** CSc1nc(N(C)C(=O)C(F)(F)F)nc(N(C(=O)C(F)(F)F)C(C)C)n1  
**Mol. weight [g/mol]:** 405.32

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	2.422		Crippen Method
mcvol	236.190	ml/mol	McGowan Method
rinpol	1727.00		NIST Webbook
rinpol	1727.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U373448&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/120-805-4/N-Isopropyl-N-methyl-N-N-bis-trifluoroacetyl-6-methylsulfanyl-1-3-5-triazine-2,4-diamine>

Generated by Cheméo on 2024-04-29 11:42:43.002079139 +0000 UTC m=+16680211.922656461.  
Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.