

1,3,5-Triazine, 2,4,6-tris(trifluoromethyl)-

Other names:	s-Triazine, 2,4,6-tris(trifluoromethyl)- 2,4,6-Tris(trifluoromethyl)-s-triazine 2,4,6-Tris(trifluoromethyl)-1,3,5-triazine TTT
Inchi:	InChI=1S/C6F9N3/c7-4(8,9)1-16-2(5(10,11)12)18-3(17-1)6(13,14)15
InchiKey:	LSGBKABSSSIRJF-UHFFFAOYSA-N
Formula:	C6F9N3
SMILES:	FC(F)(F)c1nc(C(F)(F)F)nc(C(F)(F)F)n1
Mol. weight [g/mol]:	285.07
CAS:	368-66-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	2.928		Crippen Method
mcvol	117.510	ml/mol	McGowan Method
tb	368.00	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C368661&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

Latest version available from:

<https://www.chemeo.com/cid/10-026-1/1-3-5-Triazine-2-4-6-tris-trifluoromethyl.pdf>

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