

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

Other names:	s-Triazine, 2,4,6-tris(heptafluoropropyl)- 2,4,6-Tris-(heptafluoropropyl)-1,3,5-triazine Tris(perfluoropropyl)-S-triazine Tris(heptafluoropropyl)-s-triazine
Inchi:	InChI=1S/C12F21N3/c13-4(14,7(19,20)10(25,26)27)1-34-2(5(15,16)8(21,22)11(28,29)30
InchiKey:	KXQUYHRRCVECPV-UHFFFAOYSA-N
Formula:	C12F21N3
SMILES:	FC(F)(F)C(F)(F)C(F)(F)c1nc(C(F)(F)C(F)(F)C(F)(F)F)nc(C(F)(F)C(F)(F)C(F)(F)F)n1
Mol. weight [g/mol]:	585.12
CAS:	915-76-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.48		Crippen Method
logp	6.740		Crippen Method
mcvol	223.290	ml/mol	McGowan Method
tb	438.00	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C915764&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	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
tb:	Normal Boiling Point Temperature

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<https://www.chemeo.com/cid/16-457-7/1-3-5-Triazine-2-4-6-tris-heptafluoropropyl.pdf>

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