

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

Other names:	s-Triazine, 2,4,6-tris(pentafluoroethyl)- 2,4,6-Tris(pentafluoroethyl)-1,3,5-triazine Tris(perfluoroethyl)-S-triazine Tris(pentafluoroethyl)-s-triazine
Inchi:	InChI=1S/C9F15N3/c10-4(11,7(16,17)18)1-25-2(5(12,13)8(19,20)21)27-3(26-1)6(14,15)9
InchiKey:	MQBPAXAOMVELQG-UHFFFAOYSA-N
Formula:	C9F15N3
SMILES:	FC(F)(F)C(F)(F)c1nc(C(F)(F)C(F)(F)F)nc(C(F)(F)C(F)(F)F)n1
Mol. weight [g/mol]:	435.09
CAS:	858-46-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.28		Crippen Method
logp	4.834		Crippen Method
mcvol	170.400	ml/mol	McGowan Method
tb	394.50 ± 0.50	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C858468&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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