1,3,5-Triazine, 2,4,6-trifluoro-

Other names:	2,4,6-Trifluoro-1,3,5-triazine
	2,4,6-Trifluoro-s-triazine
	2,4,6-Trifluorotriazine
	Cyanuric fluoride
	Cyanuric trifluoride
	Trifluoro-1,3,5-triazine
	Trifluoro-s-triazine
	Trifluorotriazine
	s-Triazine, 2,4,6-trifluoro-
Inchi:	InChI=1S/C3F3N3/c4-1-7-2(5)9-3(6)8-1
InchiKey:	VMKJWLXVLHBJNK-UHFFFAOYSA-N
Formula:	C3F3N3
SMILES:	Fc1nc(F)nc(F)n1
Mol. weight [g/mol]:	135.05
CAS:	675-14-9

Physical Properties

Property code	Value	Unit	Source
ie	11.30	eV	NIST Webbook
ie	11.50	eV	NIST Webbook
ie	12.30	eV	NIST Webbook
log10ws	-1.76		Crippen Method
logp	0.289		Crippen Method
mcvol	64.620	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	38.80	kJ/mol	310.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51131e+01
Coeff. B	-3.04148e+03
Coeff. C	-5.60400e+01
Temperature range (K), min.	261.19
Temperature range (K), max.	366.34

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C675149&Units=SI

Legend

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure