Benzo[1,2-c:3,4-c':5,6-c'']tris[1,2,5]oxadiazole, 1,4,7-trioxide

Other names:	Benzenetrifuroxan
	Benzotrifuroxan
	Benzotris[c]furazan-2-oxide
	Benzotris[1,2,5]oxadiazole, 1,4,7-trioxide
	BTF
Inchi:	InChI=1S/C6N6O6/c13-10-4-1(7-16-10)5-3(8-17-11(5)14)6-2(4)9-18-12(6)15
InchiKey:	ROSQKRBIBODSRH-UHFFFAOYSA-N
Formula:	C6N6O6
SMILES:	[O-][n+]1onc2c1c1no[n+]([O-])c1c1no[n+]([O-])c21
Mol. weight [g/mol]:	252.10
CAS:	3470-17-5

Physical Properties

Property code	Value	Unit	Source
chs	-2967.00 ± 4.00	kJ/mol	NIST Webbook
hfs	606.00 ± 4.00	kJ/mol	NIST Webbook
log10ws	-21.97		Crippen Method
logp	-1.990		Crippen Method
mcvol	121.260	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	172.00 ± 2.50	kJ/mol	398.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3470175&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume