

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

Other names:	Benzotris[1,2,5]oxadiazole Benzotrifurazan
Inchi:	InChI=1S/C6N6O3/c7-1-2(8-13-7)4-6(12-15-11-4)5-3(1)9-14-10-5
InchiKey:	AVIIIOEOPBJOTOH-UHFFFAOYSA-N
Formula:	C6N6O3
SMILES:	n1onc2c1c1nonc1c1nonc21
Mol. weight [g/mol]:	204.10
CAS:	16279-15-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-16.68		Crippen Method
logp	0.295		Crippen Method
mcvol	103.650	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	95.80 ± 3.80	kJ/mol	318.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16279155&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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