

1,2,3-Benzotriazine-4(3h)-one, 6-nitro-

Inchi:	InChI=1S/C7H4N4O3/c12-7-5-3-4(11(13)14)1-2-6(5)8-10-9-7/h1-3H,(H,8,9,12)
InchiKey:	HFYBDBPOKYEMJB-UHFFFAOYSA-N
Formula:	C7H4N4O3
SMILES:	O=c1[nH]nnc2ccc([N+](=O)[O-])cc12
Mol. weight [g/mol]:	192.13
CAS:	91532-29-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.10		Crippen Method
logp	-0.256		Crippen Method
mcvol	119.500	ml/mol	McGowan Method

Sources

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=C91532295&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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