

Inosine, 2',3',5'-tribenzoate

Inchi:	InChI=1S/C31H24N4O8/c36-27-23-26(32-17-33-27)35(18-34-23)28-25(43-31(39)21-14-8
InchiKey:	HYIROYSRWYWYBO-UHFFFAOYSA-N
Formula:	C31H24N4O8
SMILES:	O=C(OCC1OC(n2cnc3c(=O)[nH]cnc32)C(OC(=O)c2ccccc2)C1OC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	580.54
CAS:	6741-88-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.16		Crippen Method
logp	2.843		Crippen Method
mcvol	400.570	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6741884&Units=SI

Legend

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

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<https://www.chemeo.com/cid/71-032-7/Inosine-2-3-5-tribenzoate.pdf>

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