1H-Purine-2,6-dione, 3,7-dihydro-1-methyl-3-(2-methylpropyl)-

Other names:	IBMX
	IMX
	Isobutylmethylxanthine
	3-Isobutyl-1-methylxanthine
	Methylisobutylxanthine
	1-Methyl-3-isobutylxanthine
	SC 2964
	Xanthine, 3-Isobutyl-1-methyl-
	3-Isobutyl-1-methyl-3,7-dihydro-1H-purine-2,6-dione
	Xanthine, 1-methyl-3-(2-methylpropyl)
	NSC 165960
	3,7-dihydro-3-isobutyl-1-methyl-1H-purine-2,6-dione
Inchi:	InChI=1S/C10H14N4O2/c1-6(2)4-14-8-7(11-5-12-8)9(15)13(3)10(14)16/h5-6H,4H2,1-3H
InchiKey:	APIXJSLKIYYUKG-UHFFFAOYSA-N
Formula:	C10H14N4O2
SMILES:	CC(C)Cn1c(=O)n(C)c(=O)c2[nH]cnc21
Mol. weight [g/mol]:	222.24
CAS:	28822-58-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	-0.403		Crippen Method
mcvol	164.500	ml/mol	McGowan Method
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook

Sources

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=C28822584&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices