N-(2-Hydroxyethyl)-4-cyclohexene-1,2-dicarboxim

Other names:	N-(«beta»-Hydroxyethyl)-4-cyclohexen-1,2-dicarboximide
	N-(«beta»-Hydroxyethyl)-4-cyclohexene-1,2-dicarboximide
	1H-Isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-2-(2-hydroxyethyl)-
	1,2,3,6,-tetrahydro-N-(2-hydroxyethyl)phthalimide
Inchi:	InChI=1S/C10H13NO3/c12-6-5-11-9(13)7-3-1-2-4-8(7)10(11)14/h1-2,7-8,12H,3-6H2
InchiKey:	MRADHZSVGNCOQU-UHFFFAOYSA-N
Formula:	C10H13NO3
SMILES:	O=C1C2CC=CCC2C(=O)N1CCO
Mol. weight [g/mol]:	195.22
CAS:	15458-48-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.55		Crippen Method
logp	-0.070		Crippen Method
mcvol	144.730	ml/mol	McGowan Method

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=C15458487&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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