1,2-Cyclobutane-dicarboximide, n-ethyl-4-dimethylamino-3,3-dimethyl-

Inchi: InChI=1S/C12H20N2O2/c1-6-14-10(15)7-8(11(14)16)12(2,3)9(7)13(4)5/h7-9H,6H2,1-5H3

InchiKey: NZBAPHBJUSRLAC-UHFFFAOYSA-N

Formula: C12H20N2O2

SMILES: CCN1C(=O)C2C(C1=O)C(C)(C)C2N(C)C

Mol. weight [g/mol]: 224.30

CAS: 91638-02-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.71		Crippen Method
logp	0.578		Crippen Method
mcvol	181.320	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=C91638027&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