Diethyl piperazine-1,4-dicarboxylate

Inchi: InChI=1S/C10H18N2O4/c1-3-15-9(13)11-5-7-12(8-6-11)10(14)16-4-2/h3-8H2,1-2H3
InchiKey: NAEAAGULDNVNCW-UHFFFAOYSA-N
Formula: C10H18N2O4
SMILES: CCOC(=O)N1CCN(C(=O)OCC)CC1
Mol. weight [g/mol]: 230.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.73		Aqueous Solubility Prediction Method
logp	0.917		Crippen Method
mcvol	175.740	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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