Benzoic acid, p-[(2-hydroxy-3-phthalimidopropyl)amino]-, ethyl ester

InChI: InChI=1S/C20H20N2O5/c1-2-27-20(26)13-7-9-14(10-8-13)21-11-15(23)12-22-18(24)16-5
InchiKey: XKIALGNRNRCYFX-UHFFFAOYSA-N
Formula: C20H20N2O5
SMILES: CCOC(=O)c1ccc(NCC(O)CN2C(=O)c3ccccc3C2=O)cc1
Mol. weight [g/mol]: 368.38
CAS: 132854-37-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.94		Crippen Method
logp	1.932		Crippen Method
mcvol	270.690	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=C132854376&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

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