D-N-Benzyl tartarimide

Inchi: InChI=1S/C11H11NO4/c13-8-9(14)11(16)12(10(8)15)6-7-4-2-1-3-5-7/h1-5,8-9,13-14H,6H
InchiKey: IZBMPGFJNIDMRR-UHFFFAOYSA-N
Formula: C11H11NO4
SMILES: O=C1C(O)C(O)C(=O)N1Cc1ccccc1
Mol. weight [g/mol]: 221.21
CAS: 19728-93-9

Physical Properties

Property code	Value	Unit	Source
chs	-5182.42	kJ/mol	NIST Webbook
log10ws	-0.79		Crippen Method
logp	-0.723		Crippen Method
mcvol	156.090	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=C19728939&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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