5-BENZYLOXYINDOLE-2-CARBOXYLIC ACID

Other names: 1H-Indole-2-carboxylic acid, 5-(phenylmethoxy)-
5-(phenylmethoxy)-1H-indole-2-carboxylic acid
Inchi: InChI=1S/C16H13NO3/c18-16(19)15-9-12-8-13(6-7-14(12)17-15)20-10-11-4-2-1-3-5-11/h
InchiKey: MVCLSAMNMAWXFQ-UHFFFAOYSA-N
Formula: C16H13NO3
SMILES: O=C(O)c1cc2cc(OCc3ccccc3)ccc2[nH]1
Mol. weight [g/mol]: 267.28

Physical Properties

Property code	Value	Unit	Source
ie	7.72	eV	Cheméo Relay (1.0)
logp	2.963		Crippen Method
mcvol	196.910	ml/mol	McGowan Method
tb	691.17	K	Cheméo Relay (1.0)
tf	506.13	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6640091&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point