

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/
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.cheméo.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

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