1H-Benzimidazole-2-acetonitrile,«alpha»-(phenylm

Inchi: InChI=1S/C16H11N3/c17-11-13(10-12-6-2-1-3-7-12)16-18-14-8-4-5-9-15(14)19-16/h1-10
InchiKey: YASZPDZHYPEICO-JLHYYAGUSA-N
Formula: C16H11N3
SMILES: N#CC(=Cc1ccccc1)c1nc2ccccc2[nH]1
Mol. weight [g/mol]: 245.28
CAS: 57319-66-1

Physical Properties

Property code	Value	Unit	Source
chl	-8230.30	kJ/mol	NIST Webbook
hfl	362.00	kJ/mol	NIST Webbook
log10ws	-5.15		Crippen Method
logp	3.145		Crippen Method
mcvol	190.660	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C57319661&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
hfl: Liquid phase enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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