

1H-Benzimidazol-2-acetonitrile, «alpha» ([4-nitroph

Inchi: InChI=1S/C16H10N4O2/c17-10-12(9-11-5-7-13(8-6-11)20(21)22)16-18-14-3-1-2-4-15(14)
InchiKey: ZTVALRSSNNLXKO-FMIVXFBMSA-N
Formula: C16H10N4O2
SMILES: N#CC(=Cc1ccc([N+](=O)[O-])cc1)c1nc2ccccc2[nH]1
Mol. weight [g/mol]: 290.28
CAS: 57319-67-2

Physical Properties

Property code	Value	Unit	Source
chl	-8007.80	kJ/mol	NIST Webbook
hfl	282.30	kJ/mol	NIST Webbook
log10ws	-5.80		Crippen Method
logp	3.053		Crippen Method
mcvol	208.080	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C57319672&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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