

# 1H-Benzimidazol-2-acetonitrile,a-([2-chlorophenyl

**Inchi:** InChI=1S/C16H10ClN3/c17-13-6-2-1-5-11(13)9-12(10-18)16-19-14-7-3-4-8-15(14)20-16/  
**InchiKey:** BPSIMQTUJJIVOO-FMIVXFBMSA-N  
**Formula:** C16H10ClN3  
**SMILES:** N#CC(=Cc1cccc1Cl)c1nc2cccc2[nH]1  
**Mol. weight [g/mol]:** 279.72  
**CAS:** 63052-08-4

## Physical Properties

Property code	Value	Unit	Source
chl	-8073.40	kJ/mol	NIST Webbook
hfl	412.80	kJ/mol	NIST Webbook
log10ws	-5.84		Crippen Method
logp	3.799		Crippen Method
mcvol	202.900	ml/mol	McGowan Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C63052084&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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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