

# Bromo-DragonFLY

**Other names:** 1-(8-Bromo-dibenzo[1,2-b; 4,5-b']difuran-4-yl-2-aminopropane  
**Inchi:** InChI=1S/C13H12BrNO2/c1-7(15)6-10-8-2-4-17-13(8)11(14)9-3-5-16-12(9)10/h2-5,7H,6,  
**InchiKey:** GIKPTWKWYXCBEU-UHFFFAOYSA-N  
**Formula:** C13H12BrNO2  
**SMILES:** CC(N)Cc1c2ccoc2c(Br)c2ccoc12  
**Mol. weight [g/mol]:** 294.14  
**CAS:** 219986-78-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-14.48		Crippen Method
logp	3.831		Crippen Method
mcvol	179.170	ml/mol	McGowan Method
rinpol	2038.00		NIST Webbook
rinpol	2087.00		NIST Webbook
rinpol	2038.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C219986784&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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