

## **Solubility Panel - Test data**

25 molecules and their aqueous solubilities in logarithmic units of mol/L

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

-1.96

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

+0.48

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

-2.11

Bergstrom CAS, Wassvik CM, et al. J Chem Inf Comput Sci, 44:1477–1488 (2004)

-3.24

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

-3.09

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

-2.64

Shareef A, Angove MJ, Wells JD, Johnson BB. J Chem Eng Data, 51:879–881 (2006)

-5.32

Bergstrom CAS, Wassvik CM, et al. J Chem Inf Comput Sci, 44:1477-1488 (2004)

-3.13

### 5-fluorouracil

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

-1.03

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

-3.25

# N H F

### fluometuron

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

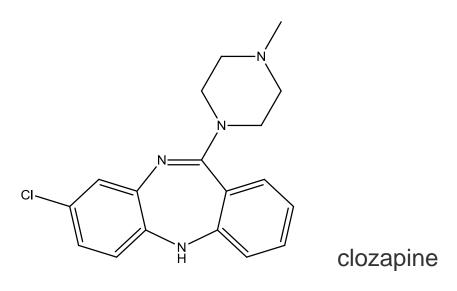
-3.46

Bergstrom CAS, Wassvik CM, et al. J Chem Inf Comput Sci, 44:1477-1488 (2004)

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

-3.02

-1.80



Hopfinger AJ, Esposito EX, et al. J Chem Inf Model, 49:1-5 (2008)

-3.24

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

-4.63

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

-0.85

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

-4.16

Palmer DS, Llinas A, Morao I, Day GM, et al. Mol Pharmaceutics, 5:266-279 (2008)

+0.02

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

-1.84

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

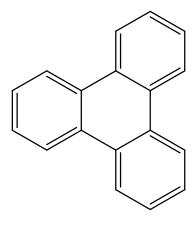
-1.36

Narasimham LYS, Barhate VD. J Pharmacy Res, 4:532-536 (2011)

-4.29

Bergstrom CAS, Luthman K, Artursson P. Eur J Pharm Sci, 22:387–398 (2004)

-5.20



### triphenylene

Rytting E, Lentz KA, Chen XQQ, Qian F, Vakatesh S. AAPS J, 7:E78-E105 (2005)

-6.73

Bergstrom CAS, Luthman K, Artursson P. Eur J Pharm Sci, 22:387–398 (2004)

-5.90