

1 (more active) or 0 (less active)

Classification
model

Difference
fingerprint

(-1 0 0 0 1 0 0 ...)

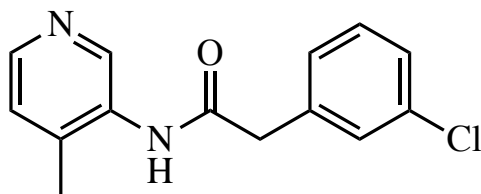
Pharmacophore
fingerprint

(0 0 1 0 1 0 1 ...)

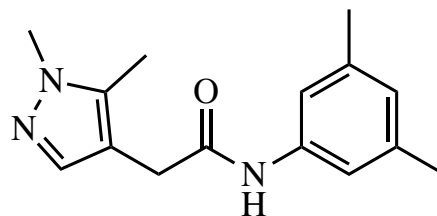
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(1 0 1 0 0 0 1 ...)

Molecular
structure



$IC_{50} = 24.6 \mu M$



$IC_{50} > 50 \mu M$