

# Nalmefene, bis(trifluoroacetate)

**Inchi:** InChI=1S/C25H23F6NO5/c1-12-6-7-23(37-21(34)25(29,30)31)16-10-14-4-5-15(35-20(33)  
**InchiKey:** JRLPCVZIWVNSEE-UHFFFAOYSA-N  
**Formula:** C25H23F6NO5  
**SMILES:** C=C1CCC2(OC(=O)C(F)(F)F)C3Cc4ccc(OC(=O)C(F)(F)F)c5c4C2(CCN3CC2CC2)C1O5  
**Mol. weight [g/mol]:** 531.44

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.39		Crippen Method
logp	4.388		Crippen Method
mcvol	322.100	ml/mol	McGowan Method
rinpola	2411.00		NIST Webbook

## Sources

**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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375689&Units=SI>

## Legend

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

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