

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/ci990307l>
Crippen Method: 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

Latest version available from:

<https://www.chemeo.com/cid/58-296-0/Nalmefene-bis-trifluoroacetate.pdf>

Generated by Cheméo on 2024-04-18 14:52:12.156940074 +0000 UTC m=+15741181.077517386.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.