

Cinepazet

Inchi: InChI=1S/C20H28N2O6/c1-5-28-19(24)14-21-8-10-22(11-9-21)18(23)7-6-15-12-16(25-2)
InchiKey: XDUOTWNXVDBCDY-SREVYHEPSA-N
Formula: C20H28N2O6
SMILES: CCOC(=O)CN1CCN(C(=O)C=Cc2cc(OC)c(OC)c(OC)c2)CC1
Mol. weight [g/mol]: 392.45
CAS: 23887-41-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Crippen Method
logp	1.433		Crippen Method
mcvol	300.320	ml/mol	McGowan Method
rinpola	2924.00		NIST Webbook
rinpola	2924.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C23887414&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: 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
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/63-277-5/Cinepazet.pdf>

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