Mofebutazone, bis-methylated

Inchi: InChI=1S/C15H20N2O2/c1-4-5-11-13-14(18-2)16-17(15(13)19-3)12-9-7-6-8-10-12/h6-10
InchiKey: JNKMMBSNMMOYNB-UHFFFAOYSA-N
Formula: C15H20N2O2
SMILES: CCCCc1c(OC)nn(-c2ccccc2)c1OC
Mol. weight [g/mol]: 260.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	3.232		Crippen Method
mcvol	210.690	ml/mol	McGowan Method
rinpol	1955.00		NIST Webbook
rinpol	1955.00		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=R201784&Units=SI

Legend

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

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