Mofebutazone, hydroxy, bis-methylated

Inchi: InChI=1S/C15H20N2O3/c1-4-5-6-13-14(18)16-17(15(13)20-3)11-7-9-12(19-2)10-8-11/h7
InchiKey: SMXNDQBABUPZCI-UHFFFAOYSA-N
Formula: C15H20N2O3
SMILES: CCCCc1c(OC)n(-c2ccc(OC)cc2)[nH]c1=O
Mol. weight [g/mol]: 276.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.64		Crippen Method
logp	2.043		Crippen Method
mcvol	216.560	ml/mol	McGowan Method
rinpol	2075.00		NIST Webbook
rinpol	2075.00		NIST Webbook

Sources

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=R201799&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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