Kebuzone, hydroxy, bis-methylated

Inchi: InChI=1S/C21H22N2O4/c1-15(24)9-14-19-20(25)22(16-7-5-4-6-8-16)23(21(19)27-3)17-1
InchiKey: QGSSTWPPDCAZHM-UHFFFAOYSA-N
Formula: C21H22N2O4
SMILES: COc1ccc(-n2c(OC)c(CCC(C)=O)c(=O)n2-c2ccccc2)cc1
Mol. weight [g/mol]: 366.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.36		Crippen Method
logp	3.167		Crippen Method
mcvol	278.910	ml/mol	McGowan Method
rinpol	2690.00		NIST Webbook
rinpol	2690.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R201704&Units=SI
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

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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