Phenbutrazate

Other names: fenbutrazate
Inchi: InChI=1S/C23H29NO3/c1-3-21(19-10-6-4-7-11-19)23(25)27-17-15-24-14-16-26-22(18(24
InchiKey: BAQKJENAVQLANS-UHFFFAOYSA-N
Formula: C23H29NO3
SMILES: CCC(C(=O)OCCN1CCOC(c2ccccc2)C1C)c1ccccc1
Mol. weight [g/mol]: 367.48
CAS: 4378-36-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	4.185		Crippen Method
mcvol	299.840	ml/mol	McGowan Method
rinpol	2670.00		NIST Webbook
rinpol	2670.00		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=C4378363&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

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