

Chromonar

Other names:	carbocromen
Inchi:	InChI=1S/C20H27NO5/c1-5-21(6-2)11-10-17-14(4)16-9-8-15(12-18(16)26-20(17)23)25-1
InchiKey:	KLOIYEQEVSIOOO-UHFFFAOYSA-N
Formula:	C20H27NO5
SMILES:	CCOC(=O)COc1ccc2c(C)c(CCN(CC)CC)c(=O)oc2c1
Mol. weight [g/mol]:	361.43
CAS:	804-10-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.19		Crippen Method
logp	2.928		Crippen Method
mcvol	284.470	ml/mol	McGowan Method
rinpol	2853.00		NIST Webbook
rinpol	2820.00		NIST Webbook
rinpol	2853.00		NIST Webbook
rinpol	2820.00		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=C804104&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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<https://www.chemeo.com/cid/62-573-7/Chromonar.pdf>

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