

Codeine-propionyl

Other names:	Codein-propionyl Codeine propanoate Codeine, propionic ester Propionylcodeine
Inchi:	InChI=1S/C21H25NO4/c1-4-17(23)25-16-8-6-13-14-11-12-5-7-15(24-3)19-18(12)21(13,2
InchiKey:	JHXSQQORTBPDKY-UHFFFAOYSA-N
Formula:	C21H25NO4
SMILES:	CCC(=O)OC1C=CC2C3Cc4ccc(OC)c5c4C2(CCN3C)C1O5
Mol. weight [g/mol]:	355.43
CAS:	65644-90-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.72		Crippen Method
logp	2.462		Crippen Method
mcvol	264.410	ml/mol	McGowan Method
rinpol	2665.00		NIST Webbook
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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=C65644908&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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