CODEIN-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

Physical Properties

Property code	Value	Unit	Source
ie	7.88	eV	Cheméo Relay (1.0)
log10ws	-2.13		Cheméo Relay (1.0)
logp	2.462		Crippen Method
mcvol	264.410	ml/mol	McGowan Method
rinpol	2665.00		NIST Webbook
rinpol	2665.00		NIST Webbook
tf	398.78	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65644908&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point