

HEPTAFLUOROBUTYRYL-CODEINE

Other names:	Codeine mono-HFB Codeine heptafluorobutyrate
Inchi:	InChI=1S/C22H20F7NO4/c1-30-8-7-19-11-4-6-14(33-18(31)20(23,24)21(25,26)22(27,28)
InchiKey:	AVCAJQCTFAWNTJ-UHFFFAOYSA-N
Formula:	C22H20F7NO4
SMILES:	COc1ccc2c3c1OC1C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C=CC4C(C2)N(C)CCC341
Mol. weight [g/mol]:	495.39

Physical Properties

Property code	Value	Unit	Source
ie	8.24	eV	Cheméo Relay (1.0)
log10ws	-4.44		Cheméo Relay (1.0)
logp	3.885		Crippen Method
mcvol	290.890	ml/mol	McGowan Method
tf	379.08	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C66091212&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

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

tf: Normal melting (fusion) point

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