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