Indoxylbutyrate

Other names: indol-3-yl butyrate
Inchi: InChI=1S/C12H13NO2/c1-2-5-12(14)15-11-8-13-10-7-4-3-6-9(10)11/h3-4,6-8,13H,2,5H2
InchiKey: DPUSLOQBAPOARC-UHFFFAOYSA-N
Formula: C12H13NO2
SMILES: CCCC(=O)Oc1c[nH]c2ccccc12
Mol. weight [g/mol]: 203.24

Physical Properties

Property code	Value	Unit	Source
ie	7.55	eV	Cheméo Relay (1.0)
log10ws	-3.51		Cheméo Relay (1.0)
logp	2.391		Crippen Method
mcvol	158.440	ml/mol	McGowan Method
tb	580.48	K	Cheméo Relay (1.0)
tf	350.90	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4346150&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

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point