

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.cheméo.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

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