

Befunolol

Inchi:	InChI=1S/C16H21NO4/c1-10(2)17-8-13(19)9-20-14-6-4-5-12-7-15(11(3)18)21-16(12)14/
InchiKey:	ZPQPDBIHCBNIG-UHFFFAOYSA-N
Formula:	C16H21NO4
SMILES:	CC(=O)c1cc2cccc(OCC(O)CNC(C)C)c2o1
Mol. weight [g/mol]:	291.35
CAS:	39552-01-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.15		Cheméo Relay (1.0)
logp	2.373		Crippen Method
mcvol	226.540	ml/mol	McGowan Method
tf	388.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

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):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637

Legend

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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<https://www.chemeo.com/cid/106-091-3/Befunolol.pdf>

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