BITERTANOL

Other names:	1H-1,2,4-Triazole-1-ethanol, «beta»-([1,1'-biphenyl]-4-yloxy)-«alpha»-(1,1-dimethylethyl)- Baycor Baymat-spray Biloxazol «beta»-((1,1'-Biphenyl)-4-yloxy)-«alpha»-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol KWG 0599 Sibutol BAY KWG 0599 1-([1,1'-Biphenyl]-4-yloxy)-3,3-dimethyl-1-(1H-1,2,4-triazol-1-yl)-2-butanol Baycor 25 WP «beta»-([1,1'-biphenyl]-4-yloxy)-«alpha»-tert-butyl-1H-1,2,4-triazol-1-ethanol
Inchi:	InChI=1S/C20H23N3O2/c1-20(2,3)18(24)19(23-14-21-13-22-23)25-17-11-9-16(10-12-17
InchiKey:	VGPIBGGRCVEHQZ-UHFFFAOYSA-N
Formula:	C20H23N3O2
SMILES:	CC(C)(C)C(O)C(Oc1ccc(-c2ccccc2)cc1)n1cncn1
Mol. weight [g/mol]:	337.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.25		Cheméo Relay (1.0)
logp	3.930		Crippen Method
mcvol	267.360	ml/mol	McGowan Method
tf	427.93	K	Cheméo Relay (1.0)

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55179312&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point