Paclobutrazol

Other names:

(2RS,3RS)-1-(4-Chlorophenyl)-4,4-dimethyl-2-(1H-1,2,4-triazol-1-yl)pentan-3-ol
(2S,3S)-1-(4-chlorophenyl)-4,4-dimethyl-2-(1H-1,2,4-triazol-1-yl)pentan-3-ol
(R*,R*)-(.+/-.)-«beta»-[(4-Chlorophenyl)methyl]-«alpha»-(1,1dimethylethyl)-1H-1,2,4-triazo
1-(4-Chlorophenyl)-4,4-dimethyl-2-(1H-1,2,4-triazol-1-yl)-3-pentanol, (2RS,3RS)-
1H-1,2,4-Triazole-1-ethanol,
beta-((4-chlorophenyl)methyl)-«alpha»-(1,1-dimethylethyl)-, (R*,R*)-
1H-1,2,4-Triazole-1-ethanol,
beta-((4-chlorophenyl)methyl)-«alpha»-(1,1-dimethylethyl)-, (R*,R*)-(.+/-.)-
1H-1,2,4-Triazole-1-ethanol,
beta-((4-chlorophenyl)methyl)-«alpha»-(1,1-dimethylethyl)-,
(«alpha»R,«beta»R)-rel-
«beta»-[(4-chlorophenyl)methyl]-«alpha»-(1,1-dimethylethyl)-,
(«alpha»R,«beta»R)-rel-
2S,3S-Paclobutrazol
Bonsai
Bonzi
Bounty flowable
Clipper
Cultar
Duo Xiao Zuo
Friazole
ICI-PP-333
PP 333
Paclobutrazole
Parlay
Smarect
Trimmit

Inchi:

«beta»-((4-Chlorophenyl)methyl)-«alpha»-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol,
(R*,R*)-(.+/-.)-
InChI=1S/C15H20ClN3O/c1-15(2,3)14(20)13(19-10-17-9-18-19)8-11-4-6-12(16)7-5-11/h

InchiKey: RMOGWMIKYWRTKW-UHFFFAOYSA-N
Formula: C15H20ClN3O
SMILES: CC(C)(C)C(O)C(Cc1ccc(Cl)cc1)n1cncn1
Mol. weight [g/mol]: 293.79
CAS: 76738-62-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.75		Crippen Method
logp	3.122		Crippen Method
mcvol	227.040	ml/mol	McGowan Method
rinpol	2128.00		NIST Webbook

tf	433.81	K	Solubility determination and thermodynamic modeling of paclobutrazol in nine organic solvents from T = (278.15 to 318.15) K and mixing properties of solutions

Sources

Solubility modelling and preferential solvation of paclobutrazol in cosolvent mixtures of (ethanol, n-propanol and 1,4-dioxane) + water:	https://www.doi.org/10.1016/j.jct.2017.05.004
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76738620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility determination and thermodynamic modeling of paclobutrazol in nine organic solvents from T = (278.15 to 318.15) K and mixing properties of solutions:	https://www.doi.org/10.1016/j.jct.2016.09.038

Legend

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