Triadimenol

Other names:	Baytan
	Bayfidan
	Ethanol, 2-(4-chlorophenoxy)-1-tert-butyl-2-(1H-1,2,4-triazole-1-yl)-
	1H-1,2,4-Triazole-1-ethanol, «beta»-(4-chlorophenoxy)-«alpha»-(1,1-dimethylethyl)-
	BAY KWG 0519
	2-(4-Chlorophenoxy)-1-tert-butyl-2-(1H-1,2,4-triazole-1-yl)ethanol
	«beta»-(4-Chlorophenoxy)-«alpha»-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol
	Summit
	Spinnaker
	Bayfidan EW
	Baytan 15
	Baytan TF 3479B
	KWG 0519
	UK 199
	Triadimenol, isomer 2
	Triadimenol (2)
	Triadimenol, isomer 1
	Triadimenol (1)
	«alpha»-tert-butyl-«beta»-(4-chlorophenoxy)-1H-1,2,4-triazole-1-ethanol
Inchi:	InChI=1S/C14H18ClN3O2/c1-14(2,3)12(19)13(18-9-16-8-17-18)20-11-6-4-10(15)5-7-11/h
InchiKey:	BAZVSMNPJJMILC-UHFFFAOYSA-N
Formula:	C14H18ClN3O2
SMILES:	CC(C)(C)C(O)C(Oc1ccc(Cl)cc1)n1cncn1
Mol. weight [g/mol]:	295.76
CAS:	55219-65-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.57		Crippen Method
logp	2.916		Crippen Method
mcvol	218.820	ml/mol	McGowan Method
rinpol	2084.00		NIST Webbook
rinpol	2069.00		NIST Webbook
rinpol	2076.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2023.00		NIST Webbook
rinpol	2095.00		NIST Webbook

rinpol	2088.00		NIST Webbook
rinpol	2104.00		NIST Webbook
rinpol	2050.00		NIST Webbook
tf	380.99 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	24.47	kJ/mol	377.80	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55219653&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfust: Enthalpy of fusion at a given temperature
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