Myclobutanil

Other names: .alpha.-butyl-.alpha.-(4-chlorophenyl)-1H-1,2,4-triazole-1-propanenitrile
1H-1,2,4-Triazole-1-propanenitrile, «alpha»-butyl-«alpha»-(4-chlorophenyl)-
2-((1H-1,2,4-triazol-1-yl)methyl)-2-(4-chlorophenyl)hexanenitrile
Nova
RH-3866
Rally
Systhane
a-butyl-a-(4-chlorophenyl)-1H-1,2,4-triazole-1-propanenitrile
«alpha»-butyl-«alpha»-(4-chlorophenyl)-1H-1,2,4-triazole-1-propanenitrile
«alpha»-butyl-«alpha»-(4-chlorophenyl)-1H-1,2,4-triazole-1-propanenitrile
(myclobutanil)

Inchi: InChI=1S/C15H17ClN4/c1-2-3-8-15(9-17,10-20-12-18-11-19-20)13-4-6-14(16)7-5-13/h4-

InchiKey: HZJKXKUJVSEEFU-UHFFFAOYSA-N

Formula: C15H17ClN4

SMILES: CCCCC(C#N)(Cn1cncn1)c1ccc(Cl)cc1

Mol. weight [g/mol]: 288.77

CAS: 88671-89-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.20		Crippen Method
logp	3.583		Crippen Method
mcvol	222.550	ml/mol	McGowan Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2198.00		NIST Webbook
rinpol	2198.00		NIST Webbook
tf	343.45	K	Crystal structure and thermodynamic properties of myclobutanil

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	30.93	kJ/mol	348.80	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crystal structure and thermodynamic properties of myclobutanil:	https://www.doi.org/10.1016/j.jct.2016.05.014
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88671890&Units=SI

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