

Metazachlor

Other names:

Acetamide, 2-chloro-N-(2,6-dimethylphenyl)-N-(1H-pyrazol-1-ylmethyl)-
BAS 479H
Butisan S
2-Chloro-N-(2,6-dimethylphenyl)-N-(1H-pyrazol-1-ylmethyl)-acetamide
Metazachlore
2-Chloro-N-(pyrazol-1-ylmethyl)acet-2',6'-xylidide
BAS 47900H
Butisan
Pree
Metazochlor

Inchi:

InChI=1S/C14H16ClN3O/c1-11-5-3-6-12(2)14(11)18(13(19)9-15)10-17-8-4-7-16-17/h3-8

InchiKey:

STEPQTYSZVCJPV-UHFFFAOYSA-N

Formula:

C14H16ClN3O

SMILES:

Cc1ccc(C)c1N(Cn1cccn1)C(=O)CCl

Mol. weight [g/mol]:

277.75

CAS:

67129-08-2

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.01 | | Crippen Method |
| logp | 2.729 | | Crippen Method |
| mcvol | 208.650 | ml/mol | McGowan Method |
| rinpole | 2039.00 | | NIST Webbook |
| rinpole | 2046.00 | | NIST Webbook |
| rinpole | 2039.00 | | NIST Webbook |

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C67129082&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| rinpol: | Non-polar retention indices |

Latest version available from:

<https://www.cheméo.com/cid/119-440-1/Metazachlor.pdf>

Generated by Cheméo on 2024-05-02 04:15:49.101498998 +0000 UTC m=+16912598.022076313.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.