

Bromacil

Other names:

2,4(1H,3H)-Pyrimidinedione, 5-bromo-6-methyl-3-(1-methylpropyl)-
3-sec-Butyl-5-bromo-6-methyluracil
3-sec-Butyl-5-brom-6-methyluracil
5-Bromo-3-sec-butyl-6-methyluracil
5-Bromo-6-methyl-3-(1-methylpropyl)-2,4(1H,3H)-pyrimidinedione
5-Bromo-6-methyl-3-(1-methylpropyl)uracil
5-bromo-3-butan-2-yl-6-methyl-1H-pyrimidine-2,4-dione
Borea
Bromax
Bromazil
Croptex onyx
Cynogan
Du Pont herbicide 976
Eerex granular weed killer
Eerex water soluble concentrate weed killer
Herbicide 976
Hyvar
Hyvar X
Hyvar X Weed Killer
Hyvar X bromacil
Hyvar X-L
Hyvar X-WS
Hyvarex
Krovar II
Nalkil
Rokar X
Uracil, 5-bromo-3-sec-butyl-6-methyl-
Uragan
Uragon
Urox B
Urox B water soluble concentrate weed killer
Urox hx granular weed killer
Urox-hx

Inchi:

InChI=1S/C9H13BrN2O2/c1-4-5(2)12-8(13)7(10)6(3)11-9(12)14/h5H,4H2,1-3H3,(H,11,14)

InchiKey:

CTSLUCNDVMMDHG-UHFFFAOYSA-N

Formula:

C9H13BrN2O2

SMILES:

CCC(C)n1c(=O)[nH]c(C)c(Br)c1=O

Mol. weight [g/mol]:

261.12

CAS:

314-40-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Aqueous Solubility Prediction Method
log10ws	-2.52		Estimated Solubility Method
logp	1.097		Crippen Method
mcvol	163.110	ml/mol	McGowan Method
rinpol	1954.00		NIST Webbook
tf	430.92 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	22.02	kJ/mol	428.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C314409&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

Latest version available from:

<https://www.chemeo.com/cid/10-904-6/Bromacil.pdf>

Generated by Cheméo on 2025-12-20 04:00:26.236658479 +0000 UTC m=+5951423.766699143.

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