

Lenacil

Other names:

1H-Cyclopentapyrimidine-2,4(3H,5H)-dione, 3-cyclohexyl-6,7-dihydro-
1H-Cyclopentapyrimidine-2,4(3H,5H)-dione, 6,7-dihydro-3-cyclohexyl-
3-Cyclohexyl-1,5,6,7-tetrahydro-2H-cyclopentapyrimidine-2,4(3H)-dione
3-Cyclohexyl-1,5,6,7-tetrahydrocyclopentapyrimidine-2,4(3H)-dione
3-Cyclohexyl-5,6-trimethylenuracil
3-Cyclohexyl-5,6-trimethylenuracil
3-Cyclohexyl-6,7-dihydro-1H-cyclopentapyrimidine-2,4-(3H,5H)-dione
Adol
Adol (pesticide)
Buracyl
Du Pont 634
Elbatan
Experimental Herbicide 634
Herbicide 634
Hexilure
Lenacile
Uracil 634
Venzar
Vizor

Inchi:

InChI=1S/C13H18N2O2/c16-12-10-7-4-8-11(10)14-13(17)15(12)9-5-2-1-3-6-9/h9H,1-8H2

InchiKey:

ZTMKADLOSJKWCA-UHFFFAOYSA-N

Formula:

C13H18N2O2

SMILES:

O=c1c2c(nc(O)n1C1CCCC1)CCC2

Mol. weight [g/mol]:

234.29

CAS:

2164-08-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Aqueous Solubility Prediction Method
log10ws	-4.59		Estimated Solubility Method
logp	1.943		Crippen Method
mcvol	180.250	ml/mol	McGowan Method
rinpol	2276.00		NIST Webbook
rinpol	2359.00		NIST Webbook
tf	584.55 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	42.31	kJ/mol	584.30	NIST Webbook

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2164081&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

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