

Hexazinone

Other names:

1,3,5-Triazine-2,4(1H,3H)-dione, 3-cyclohexyl-6-(dimethylamino)-1-methyl-
3-Cyclohexyl-1-methyl-6-(dimethylamino)-s-triazine-2,4(1H,3H)-dione
s-Triazine-2,4(1H,3H)-dione, 3-cyclohexyl-6-(dimethylamino)-1-methyl-
3-Cyclohexyl-6-(dimethylamino)-1-methyl-s-triazine-2,4(1H,3H)-dione
3-Cyclohexyl-6-(dimethylamino)-1-methyl-1,3,5-triazine-2,4(1H,3H)-dione
DPX 3674
Velpar
Velpar weed killer
3-Cyclohexy-6-(dimethylamino)-1-methyl-1,3,5-triazine-2,4(1H,3H)-dione
Hexazinon
Velpar L
3-cyclohexyl-6-dimethylamino-1-methyl-1,2,3,4-tetrahydro-1,3,5-triazine-2,4-dione

Inchi: InChI=1S/C12H20N4O2/c1-14(2)10-13-11(17)16(12(18)15(10)3)9-7-5-4-6-8-9/h9H,4-8H2
InchiKey: CAWXEEYDBZRFPE-UHFFFAOYSA-N
Formula: C12H20N4O2
SMILES: CN(C)c1nc(=O)n(C2CCCCC2)c(=O)n1C
Mol. weight [g/mol]: 252.31
CAS: 51235-04-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.07		Crippen Method
logp	0.513		Crippen Method
mcvol	196.980	ml/mol	McGowan Method
rinpol	2380.00		NIST Webbook
rinpol	2381.00		NIST Webbook
tf	390.35 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.36	kJ/mol	389.60	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51235042&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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