2,4(1H,3H)-Pyrimidinedione, 6-phenyl-

Other names:	6-Phenyl-2,4(1H,3H)-pyrimidinedione
	6-Phenyluracil
Inchi:	InChI=1S/C10H8N2O2/c13-9-6-8(11-10(14)12-9)7-4-2-1-3-5-7/h1-6H,(H2,11,12,13,14)
InchiKey:	NCSMAVULYUCSMB-UHFFFAOYSA-N
Formula:	C10H8N2O2
SMILES:	O=c1cc(-c2ccccc2)[nH]c(=O)[nH]1
Mol. weight [g/mol]:	188.18
CAS:	13345-09-0

Physical Properties

Property code	Value	Unit	Source
chs	-4748.40	kJ/mol	NIST Webbook
chs	-4748.40	kJ/mol	NIST Webbook
log10ws	-1.36		Crippen Method
logp	-0.234		Crippen Method
mcvol	135.940	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13345090&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume