benzoyleneurea

Inchi: InChI=1S/C8H6N2O2/c11-7-5-3-1-2-4-6(5)9-8(12)10-7/h1-4H,(H2,9,10,11,12)
InchiKey: SDQJTWBNWQABLE-UHFFFAOYSA-N
Formula: C8H6N2O2
SMILES: O=c1[nH]c(=O)c2ccccc2[nH]1
Mol. weight [g/mol]: 162.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.56		Crippen Method
logp	-0.747		Crippen Method
mcvol	112.060	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	128.30 ± 3.00	kJ/mol	298.15	Energetics of Quinazoline-2,4(1H,3H)-dione: An Experimental and Computational Study

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Energetics of Quinazoline-2,4(1H,3H)-dione: An Experimental and Computational Study:	https://www.doi.org/10.1021/je2004929

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume