4-Benzoyl-3-furazanamine

Inchi: InChI=1S/C9H7N3O2/c10-9-7(11-14-12-9)8(13)6-4-2-1-3-5-6/h1-5H,(H2,10,12)
InchiKey: FSUWRFXTSWSYPV-UHFFFAOYSA-N
Formula: C9H7N3O2
SMILES: Nc1nonc1C(=O)c1ccccc1
Mol. weight [g/mol]: 189.17
CAS: 38924-53-7

Physical Properties

Property code	Value	Unit	Source
chs	-4621.20 ± 5.00	kJ/mol	NIST Webbook
log10ws	-6.33		Crippen Method
logp	0.883		Crippen Method
mcvol	131.830	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38924537&Units=SI

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

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