

N-Nitrophthalamide

Inchi:	InChI=1S/C8H4N2O4/c11-7-5-3-1-2-4-6(5)8(12)9(7)10(13)14/h1-4H
InchiKey:	JKLDLZVPEFRPLS-UHFFFAOYSA-N
Formula:	C8H4N2O4
SMILES:	O=C1c2ccccc2C(=O)N1[N+](=O)[O-]
Mol. weight [g/mol]:	192.13
CAS:	5336-97-0

Physical Properties

Property code	Value	Unit	Source
chs	-3495.00	kJ/mol	NIST Webbook
log10ws	-2.48		Crippen Method
logp	0.474		Crippen Method
mcvol	119.500	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5336970&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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