N-acetyl-n-(p-phthalimidobenze-sulfonyl)-2-amino

Inchi: InChI=1S/C22H18N4O5S/c1-13-12-14(2)24-22(23-13)26(15(3)27)32(30,31)17-10-8-16(9
InchiKey: HPKTVFANTNFJNB-UHFFFAOYSA-N
Formula: C22H18N4O5S
SMILES: CC(=O)N(c1nc(C)cc(C)n1)S(=O)(=O)c1ccc(N2C(=O)c3ccccc3C2=O)cc1
Mol. weight [g/mol]: 450.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.64		Crippen Method
logp	2.636		Crippen Method
mcvol	311.420	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=B6003524&Units=SI

Legend

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