N-(4-Morpholin-4-yl-phenyl)-2-nitro-benzenesulfon-N-methyl-

Inchi: InChI=1S/C17H19N3O5S/c1-18(26(23,24)17-5-3-2-4-16(17)20(21)22)14-6-8-15(9-7-14)1

InchiKey: VDDHYVMLRUNJAP-UHFFFAOYSA-N

Formula: C17H19N3O5S

SMILES: CN(c1ccc(N2CCOCC2)cc1)S(=O)(=O)c1ccccc1[N+](=O)[O-]

Mol. weight [g/mol]: 377.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.25		Crippen Method
logp	2.256		Crippen Method
mcvol	263.350	ml/mol	McGowan Method
rinpol	3239.00		NIST Webbook
rinpol	3239.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374817&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.