

Sebacic acid, ethyl 2-(2-methyl-5-nitro-1H-imidazol-1-yl)ethyl

Inchi:
ester

InChI=1S/C18H29N3O6/c1-3-26-17(22)10-8-6-4-5-7-9-11-18(23)27-13-12-20-15(2)19-14

InchiKey:

NCHXNWPPHGUNBZ-UHFFFAOYSA-N

Formula:

C18H29N3O6

SMILES:

CCOC(=O)CCCCCCCC(=O)OCCn1c([N+](=O)[O-])cnc1C

Mol. weight [g/mol]:

383.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.37		Crippen Method
logp	3.327		Crippen Method
mcvol	297.280	ml/mol	McGowan Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.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=U380633&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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