

Phthalimide, n-[4-(tetrahydro-2-oxo-2h-1,3-oxazin-3-yl)butyl]-

Inchi: InChI=1S/C16H18N2O4/c19-14-12-6-1-2-7-13(12)15(20)18(14)10-4-3-8-17-9-5-11-22-16
InchiKey: UBZSPJWURXPKGF-UHFFFAOYSA-N
Formula: C16H18N2O4
SMILES: O=C1OCCCN1CCCCN1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]: 302.33
CAS: 23545-36-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	1.905		Crippen Method
mcvol	221.360	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C23545360&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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