

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

Inchi: InChI=1S/C15H16N2O4/c18-13-11-5-1-2-6-12(11)14(19)17(13)9-3-7-16-8-4-10-21-15(16)
InchiKey: VPRCLHRAWQSDH-UHFFFAOYSA-N
Formula: C15H16N2O4
SMILES: O=C1OCCCN1CCCN1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]: 288.30
CAS: 23545-35-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Crippen Method
logp	1.515		Crippen Method
mcvol	207.270	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=C23545359&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

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