1H,2H,3H,4H-Pyrido[2,1-b]quinazolin-11-one

Other names: 1,2,3,4-Tetrahydro-pyrido[2,1-b]quinazolin-11-one
Inchi: InChI=1S/C12H12N2O/c15-12-9-5-1-2-6-10(9)13-11-7-3-4-8-14(11)12/h3-4,7-8H,1-2,5-6
InchiKey: KIDSCEBUTHOOGI-UHFFFAOYSA-N
Formula: C12H12N2O
SMILES: O=c1c2c(nc3ccccn13)CCCC2
Mol. weight [g/mol]: 200.24
CAS: 25816-55-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	1.573		Crippen Method
mcvol	151.690	ml/mol	McGowan Method
rinpol	2064.00		NIST Webbook
rinpol	2064.00		NIST Webbook
rinpol	2064.00		NIST Webbook

Sources

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=C25816551&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices