2-[(2-aminopurin-9-yl)methoxy]ethanol

Inchi: InChI=1S/C8H11N5O2/c9-8-10-3-6-7(12-8)13(4-11-6)5-15-2-1-14/h3-4,14H,1-2,5H2,(H2
InchiKey: OKQHSIGMOWQUIK-UHFFFAOYSA-N
Formula: C8H11N5O2
SMILES: Nc1ncc2ncn(COCCO)c2n1
Mol. weight [g/mol]: 209.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.08		Aqueous Solubility Prediction Method
logp	-0.625		Crippen Method
mcvol	146.300	ml/mol	McGowan Method
tf	461.65	K	Aqueous Solubility Prediction Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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