

1-Azidopentane

Inchi: InChI=1S/C5H11N3/c1-2-3-4-5-7-8-6/h2-5H2,1H3
InchiKey: YJHBJNGBMWHOFD-UHFFFAOYSA-N
Formula: C5H11N3
SMILES: CCCCCN=[N+]=[N-]
Mol. weight [g/mol]: 113.16
CAS: 26330-06-3

Physical Properties

Property code	Value	Unit	Source
chl	-3691.00 ± 2.00	kJ/mol	NIST Webbook
hfl	151.00	kJ/mol	NIST Webbook
log10ws	-7.00		Crippen Method
logp	2.487		Crippen Method
mcvol	102.650	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=C26330063&Units=SI>

Legend

chl: Standard liquid enthalpy of combustion
hfl: Liquid phase enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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