

1,7-Cyclotridecadiyne

Inchi: InChI=1S/C13H18/c1-2-4-6-8-10-12-13-11-9-7-5-3-1/h1-5,10-13H2
InchiKey: JJCWLXCBUFGPRY-UHFFFAOYSA-N
Formula: C13H18
SMILES: C1#CCCCCCC#CCCCC1
Mol. weight [g/mol]: 174.28
CAS: 4533-25-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.75		Crippen Method
logp	3.518		Crippen Method
mcpvol	165.970	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	348.00 ± 5.00	K	0.00	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4533259&Units=SI>
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>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tbrp: Boiling point at reduced pressure

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