1,8-Cyclopentadecadiyne

Inchi: InChI=1S/C15H22/c1-2-4-6-8-10-12-14-15-13-11-9-7-5-3-1/h1-6,11-15H2
InchiKey: LLYOCFZRCOXMHY-UHFFFAOYSA-N
Formula: C15H22
SMILES: C1#CCCCCCCC#CCCCCC1
Mol. weight [g/mol]: 202.34
CAS: 4722-42-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.59		Crippen Method
logp	4.298		Crippen Method
mcvol	194.150	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.00 ± 5.00	K	0.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C4722423&Units=SI

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