OXACYCLOTETRADECA-4,11-DIYNE

Other names: Oxacyclotetradeca-4,11-dyine
Inchi: InChI=1S/C13H18O/c1-2-4-6-8-10-12-14-13-11-9-7-5-3-1/h1-5,10-13H2
InchiKey: ISEQOSOYOGJYOG-UHFFFAOYSA-N
Formula: C13H18O
SMILES: C1#CCCOCCC#CCCCCC1
Mol. weight [g/mol]: 190.29

Physical Properties

Property code	Value	Unit	Source
hf	200.69	kJ/mol	Cheméo Relay (1.0)
hvap	72.27	kJ/mol	Cheméo Relay (1.0)
ie	8.86	eV	Cheméo Relay (1.0)
log10ws	-2.12		Cheméo Relay (1.0)
logp	2.754		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2684.79	kPa	Cheméo Relay (1.0, beta)
rinpol	1639.00		NIST Webbook
rinpol	1639.00		NIST Webbook
rinpol	1639.00		NIST Webbook
tb	548.38	K	Cheméo Relay (1.0)
tc	779.60	K	Cheméo Relay (1.0)
tf	346.41	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6568327&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point