cis-1-Azobicyclo[2.2.2]octane

Inchi: InChI=1S/C16H26N2/c1-7-15(8-2-13(1)3-9-15)17-18-16-10-4-14(5-11-16)6-12-16/h13-14
InchiKey: OCHIAWVQRNYHIG-ZCXUNETKSA-N
Formula: C16H26N2
SMILES: C1CC2(N=NC34CCC(CC3)CC4)CCC1CC2
Mol. weight [g/mol]: 246.39
CAS: 78497-35-5

Physical Properties

Property code	Value	Unit	Source
hf	-29.31	kJ/mol	Joback Method
hvap	55.92	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.884		Crippen Method
mcvol	208.520	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
tb	759.20	K	Joback Method
tc	1027.15	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C78497355&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature