1-ISOTHIOCYANATO-4-(TRANS-4-PROPYL-CYCL

Other names: Benzene, 1-isothiocyanato-4-(trans-4-propylcyclohexyl)-
Inchi: InChI=1S/C16H21NS/c1-2-3-13-4-6-14(7-5-13)15-8-10-16(11-9-15)17-12-18/h8-11,13-14
InchiKey: IPCQSBSEIBDYIY-HDJSIYSDSA-N
Formula: C16H21NS
SMILES: CCC[C@H]1CC[C@H](c2ccc(N=C=S)cc2)CC1
Mol. weight [g/mol]: 259.42

Physical Properties

Property code	Value	Unit	Source
logp	5.495		Crippen Method
mcvol	219.410	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C92412674&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume