

1-ISOTHIOCYANATO-4-(TRANS-4-PROPYL-CYCLO

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

Latest version available from:

<https://www.chemeo.com/cid/82-393-5/1-ISOTHIOCYANATO-4-TRANS-4-PROPYL-CYCLOHEXYL-BENZENE.pdf>

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