

1-Isothiocyanato-4-(trans-4-propyl-cyclohexyl)benzene

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:	CCCC1CCC(c2ccc(N=C=S)cc2)CC1
Mol. weight [g/mol]:	259.41
CAS:	92412-67-4

Physical Properties

Property code	Value	Unit	Source
hf	169.54	kJ/mol	Joback Method
hvap	64.71	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.495		Crippen Method
mcvol	219.410	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
tb	757.97	K	Joback Method
tc	1015.11	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92412674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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