(5-Isothiocyanatopentyl)benzene

Inchi: InChI=1S/C12H15NS/c14-11-13-10-6-2-5-9-12-7-3-1-4-8-12/h1,3-4,7-8H,2,5-6,9-10H2
InchiKey: XTHYKVRNGUYFOS-UHFFFAOYSA-N
Formula: C12H15NS
SMILES: S=C=NCCCCCc1ccccc1
Mol. weight [g/mol]: 205.32
CAS: 133920-05-5

Physical Properties

Property code	Value	Unit	Source
hf	229.59	kJ/mol	Joback Method
hvap	55.02	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.502		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1809.70		NIST Webbook
rinpol	1809.70		NIST Webbook
tb	646.59	K	Joback Method
tc	884.37	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C133920055&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature