Benzhydryl isothiocyanate

Inchi: InChI=1S/C14H11NS/c16-11-15-14(12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1-10,14H
InchiKey: WDOSFTZMBFYTED-UHFFFAOYSA-N
Formula: C14H11NS
SMILES: S=C=NC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 225.31
CAS: 3550-21-8

Physical Properties

Property code	Value	Unit	Source
hf	419.56	kJ/mol	Joback Method
hvap	61.36	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.879		Crippen Method
mcvol	178.330	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	718.59	K	Joback Method
tc	1001.85	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3550218&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