Benzene, (3-isothiocyanatopropyl)-

Other names: 3-Phenylpropyl isothiocyanate
Inchi: InChI=1S/C10H11NS/c12-9-11-8-4-7-10-5-2-1-3-6-10/h1-3,5-6H,4,7-8H2
InchiKey: GRUOGLPIAPZLHJ-UHFFFAOYSA-N
Formula: C10H11NS
SMILES: S=C=NCCCc1ccccc1
Mol. weight [g/mol]: 177.27
CAS: 2627-27-2

Physical Properties

Property code	Value	Unit	Source
hf	270.87	kJ/mol	Joback Method
hvap	50.57	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.722		Crippen Method
mcvol	145.730	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	1579.60		NIST Webbook
rinpol	1579.60		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1522.00		NIST Webbook
ripol	2233.00		NIST Webbook
tb	600.83	K	Joback Method
tc	849.14	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2627272&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature