(4-isothiocyanatobutyl)benzene

Inchi: InChI=1S/C11H13NS/c13-10-12-9-5-4-8-11-6-2-1-3-7-11/h1-3,6-7H,4-5,8-9H2
InchiKey: CCBQOLFAKKAMLD-UHFFFAOYSA-N
Formula: C11H13NS
SMILES: S=C=NCCCCc1ccccc1
Mol. weight [g/mol]: 191.29
CAS: 61499-10-3

Physical Properties

Property code	Value	Unit	Source
hf	250.23	kJ/mol	Joback Method
hvap	52.80	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.112		Crippen Method
mcvol	159.820	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	1697.80		NIST Webbook
rinpol	1697.80		NIST Webbook
tb	623.71	K	Joback Method
tc	866.61	K	Joback Method

Sources

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=C61499103&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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