4-(2-Isothiocyanatoethyl)phenol

Inchi: InChI=1S/C9H9NOS/c11-9-3-1-8(2-4-9)5-6-10-7-12/h1-4,11H,5-6H2
InchiKey: DDWUOCNNMSTNMY-UHFFFAOYSA-N
Formula: C9H9NOS
SMILES: Oc1ccc(CCN=C=S)cc1
Mol. weight [g/mol]: 179.24
CAS: 60114-04-7

Physical Properties

Property code	Value	Unit	Source
hf	114.20	kJ/mol	Joback Method
hvap	61.36	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	2.038		Crippen Method
mcvol	137.510	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
rinpol	1805.90		NIST Webbook
rinpol	1805.90		NIST Webbook
tb	658.57	K	Joback Method
tc	921.27	K	Joback Method

Sources

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=C60114047&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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