(2-Isocyanatoethyl)benzene

Inchi: InChI=1S/C9H9NO/c11-8-10-7-6-9-4-2-1-3-5-9/h1-5H,6-7H2
InchiKey: HACRKYQRZABURO-UHFFFAOYSA-N
Formula: C9H9NO
SMILES: O=C=NCCc1ccccc1
Mol. weight [g/mol]: 147.17
CAS: 1943-82-4

Physical Properties

Property code	Value	Unit	Source
hf	2.03	kJ/mol	Joback Method
hvap	47.44	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	1.565		Crippen Method
mcvol	121.160	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	1225.40		NIST Webbook
rinpol	1225.40		NIST Webbook
tb	498.67	K	Joback Method
tc	716.07	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1943824&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