1-Chloro-4-(2-isocyanatoethyl)benzene

Inchi: InChI=1S/C9H8ClNO/c10-9-3-1-8(2-4-9)5-6-11-7-12/h1-4H,5-6H2
InchiKey: UFGOQTFPJKUOBH-UHFFFAOYSA-N
Formula: C9H8ClNO
SMILES: O=C=NCCc1ccc(Cl)cc1
Mol. weight [g/mol]: 181.62
CAS: 55121-08-9

Physical Properties

Property code	Value	Unit	Source
hf	-25.18	kJ/mol	Joback Method
hvap	52.48	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	2.218		Crippen Method
mcvol	133.400	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	1381.30		NIST Webbook
rinpol	1381.30		NIST Webbook
tb	541.08	K	Joback Method
tc	764.62	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=C55121089&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