2-(4-Chlorophenethyl) isothiocyanate

Inchi: InChI=1S/C9H8ClNS/c10-9-3-1-8(2-4-9)5-6-11-7-12/h1-4H,5-6H2
InchiKey: MRJJYUJULSZFDV-UHFFFAOYSA-N
Formula: C9H8ClNS
SMILES: S=C=NCCc1ccc(Cl)cc1
Mol. weight [g/mol]: 197.69
CAS: 17608-10-5

Physical Properties

Property code	Value	Unit	Source
hf	264.30	kJ/mol	Joback Method
hvap	53.39	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.985		Crippen Method
mcvol	143.880	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
tb	620.36	K	Joback Method
tc	878.63	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17608105&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature