3-Acetylphenylisothiocyanate

Inchi: InChI=1S/C9H7NOS/c1-7(11)8-3-2-4-9(5-8)10-6-12/h2-5H,1H3
InchiKey: RGANVWCPAAIVNN-UHFFFAOYSA-N
Formula: C9H7NOS
SMILES: CC(=O)c1cccc(N=C=S)c1
Mol. weight [g/mol]: 177.22
CAS: 3125-71-1

Physical Properties

Property code	Value	Unit	Source
hf	167.46	kJ/mol	Joback Method
hvap	55.75	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.623		Crippen Method
mcvol	133.210	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	636.80	K	Joback Method
tc	898.72	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3125711&Units=SI

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