Benzoic acid, 4-isothiocyanato-, ethyl ester

Other names: Phenylisothiocyanate, 4-ethoxycarbonyl
ethyl 4-isothiocyanatobenzoate
Inchi: InChI=1S/C10H9NO2S/c1-2-13-10(12)8-3-5-9(6-4-8)11-7-14/h3-6H,2H2,1H3
InchiKey: MLOJHUCMCKBDLV-UHFFFAOYSA-N
Formula: C10H9NO2S
SMILES: CCOC(=O)c1ccc(N=C=S)cc1
Mol. weight [g/mol]: 207.25
CAS: 1205-06-7

Physical Properties

Property code	Value	Unit	Source
hf	14.60	kJ/mol	Joback Method
hvap	60.39	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.598		Crippen Method
mcvol	153.170	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
tb	682.10	K	Joback Method
tc	933.38	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=C1205067&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