2-Isothiocyanato-3-phenyl-propionic acid ethyl ester

Inchi: InChI=1S/C12H13NO2S/c1-2-15-12(14)11(13-9-16)8-10-6-4-3-5-7-10/h3-7,11H,2,8H2,1H

InchiKey: YQTZICAZVVTABT-UHFFFAOYSA-N

Formula: C12H13NO2S

SMILES: CCOC(=O)C(Cc1ccccc1)N=C=S

Mol. weight [g/mol]: 235.30

Physical Properties

Property code	Value	Unit	Source
hf	-20.49	kJ/mol	Joback Method
hvap	63.79	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.264		Crippen Method
mcvol	181.350	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	1733.30		NIST Webbook
tb	722.44	K	Joback Method
tc	967.05	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177230&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