Isothiocyanic acid, (p-phenylazo)phenyl ester

Other names: p-Phenylazophenyl isothiocyanate
Diazene, (4-isothiocyanatophenyl)phenyl-
Inchi: InChI=1S/C13H9N3S/c17-10-14-11-6-8-13(9-7-11)16-15-12-4-2-1-3-5-12/h1-9H
InchiKey: ZTXNMMXJFVCQPD-UHFFFAOYSA-N
Formula: C13H9N3S
SMILES: S=C=Nc1ccc(N=Nc2ccccc2)cc1
Mol. weight [g/mol]: 239.30
CAS: 7612-96-6

Physical Properties

Property code	Value	Unit	Source
hf	481.23	kJ/mol	Joback Method
hvap	66.86	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.836		Crippen Method
mcvol	179.900	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
tb	850.33	K	Joback Method
tc	1147.09	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=C7612966&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