3,4-Methylenedioxyphenyl isothiocyanate

Inchi: InChI=1S/C8H5NO2S/c12-4-9-6-1-2-7-8(3-6)11-5-10-7/h1-3H,5H2
InchiKey: UVVSPZKAEJHDCY-UHFFFAOYSA-N
Formula: C8H5NO2S
SMILES: S=C=Nc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 179.20
CAS: 113504-93-1

Physical Properties

Property code	Value	Unit	Source
hf	118.35	kJ/mol	Joback Method
hvap	56.68	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.150		Crippen Method
mcvol	118.430	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	630.34	K	Joback Method
tc	903.71	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C113504931&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