3,4-Methylenedioxybenzyl isothiocyanate

Inchi: InChI=1S/C9H7NO2S/c13-5-10-4-7-1-2-8-9(3-7)12-6-11-8/h1-3H,4,6H2
InchiKey: PUJWRDBPAFJUJW-UHFFFAOYSA-N
Formula: C9H7NO2S
SMILES: S=C=NCc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 193.22
CAS: 4430-47-1

Physical Properties

Property code	Value	Unit	Source
hf	97.71	kJ/mol	Joback Method
hvap	58.91	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.018		Crippen Method
mcvol	132.520	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
tb	653.22	K	Joback Method
tc	919.76	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=C4430471&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