3,5-Dimethylphenyl isothiocyanate

Inchi: InChI=1S/C9H9NS/c1-7-3-8(2)5-9(4-7)10-6-11/h3-5H,1-2H3
InchiKey: DSMXCADWIFIJEX-UHFFFAOYSA-N
Formula: C9H9NS
SMILES: Cc1cc(C)cc(N=C=S)c1
Mol. weight [g/mol]: 163.24
CAS: 40046-30-8

Physical Properties

Property code	Value	Unit	Source
hf	268.57	kJ/mol	Joback Method
hvap	49.67	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.038		Crippen Method
mcvol	131.640	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
tb	587.91	K	Joback Method
tc	844.05	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40046308&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature