2,4,5-Trimethylphenyl isothiocyanate

Inchi: InChI=1S/C10H11NS/c1-7-4-9(3)10(11-6-12)5-8(7)2/h4-5H,1-3H3
InchiKey: STZONCTUVBZNCF-UHFFFAOYSA-N
Formula: C10H11NS
SMILES: Cc1cc(C)c(N=C=S)cc1C
Mol. weight [g/mol]: 177.27
CAS: 19241-18-0

Physical Properties

Property code	Value	Unit	Source
hf	236.46	kJ/mol	Joback Method
hvap	52.56	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.346		Crippen Method
mcvol	145.730	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	615.77	K	Joback Method
tc	867.11	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=C19241180&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