4-t-Butylphenyl isothiocyanate

Inchi: InChI=1S/C11H13NS/c1-11(2,3)9-4-6-10(7-5-9)12-8-13/h4-7H,1-3H3
InchiKey: OCGNNCBNRBTUCG-UHFFFAOYSA-N
Formula: C11H13NS
SMILES: CC(C)(C)c1ccc(N=C=S)cc1
Mol. weight [g/mol]: 191.29
CAS: 19241-24-8

Physical Properties

Property code	Value	Unit	Source
hf	230.01	kJ/mol	Joback Method
hvap	52.16	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.718		Crippen Method
mcvol	159.820	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
tb	625.46	K	Joback Method
tc	885.27	K	Joback Method

Sources

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=C19241248&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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