2,4,6-Tribromophenyl isothiocyanate

Inchi: InChI=1S/C7H2Br3NS/c8-4-1-5(9)7(11-3-12)6(10)2-4/h1-2H
InchiKey: ACYYDRJUIUJDCG-UHFFFAOYSA-N
Formula: C7H2Br3NS
SMILES: S=C=Nc1c(Br)cc(Br)cc1Br
Mol. weight [g/mol]: 371.87
CAS: 22134-11-8

Physical Properties

Property code	Value	Unit	Source
hf	377.37	kJ/mol	Joback Method
hvap	65.18	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.708		Crippen Method
mcvol	155.960	ml/mol	McGowan Method
pc	5289.26	kPa	Joback Method
tb	745.61	K	Joback Method
tc	1052.28	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22134118&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