4-Bromo-2-trifluoromethylphenyl isothiocyanate

Inchi: InChI=1S/C8H3BrF3NS/c9-5-1-2-7(13-4-14)6(3-5)8(10,11)12/h1-3H
InchiKey: GWLIKBAQYRDIID-UHFFFAOYSA-N
Formula: C8H3BrF3NS
SMILES: FC(F)(F)c1cc(Br)ccc1N=C=S
Mol. weight [g/mol]: 282.08
CAS: 206559-46-8

Physical Properties

Property code	Value	Unit	Source
hf	-281.54	kJ/mol	Joback Method
hvap	50.13	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.202		Crippen Method
mcvol	140.360	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
tb	625.77	K	Joback Method
tc	877.27	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=C206559468&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