4-Bromo-2,6-dimethylphenyl isothiocyanate

Inchi: InChI=1S/C9H8BrNS/c1-6-3-8(10)4-7(2)9(6)11-5-12/h3-4H,1-2H3
InchiKey: CAANWLMQHPUROR-UHFFFAOYSA-N
Formula: C9H8BrNS
SMILES: Cc1cc(Br)cc(C)c1N=C=S
Mol. weight [g/mol]: 242.14
CAS: 77159-76-3

Physical Properties

Property code	Value	Unit	Source
hf	283.43	kJ/mol	Joback Method
hvap	56.77	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.800		Crippen Method
mcvol	149.140	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
tb	659.05	K	Joback Method
tc	928.74	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77159763&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