Isothiocyanic acid, 4-bromo-3-chlorophenyl ester

Other names: 4-Bromo-3-chlorophenyl isothiocyanate
Inchi: InChI=1S/C7H3BrClNS/c8-6-2-1-5(10-4-11)3-7(6)9/h1-3H
InchiKey: NYJNWHXQEZOISL-UHFFFAOYSA-N
Formula: C7H3BrClNS
SMILES: S=C=Nc1ccc(Br)c(Cl)c1
Mol. weight [g/mol]: 248.53
CAS: 32118-33-5

Physical Properties

Property code	Value	Unit	Source
hf	320.44	kJ/mol	Joback Method
hvap	56.04	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.837		Crippen Method
mcvol	133.200	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
tb	645.74	K	Joback Method
tc	931.18	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=C32118335&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