4-Bromo-3-chlorophenyl isothiocyanate

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

Physical Properties

Property code	Value	Unit	Source
ie	8.52	eV	Cheméo Relay (1.0)
logp	3.837		Crippen Method
mcvol	133.200	ml/mol	McGowan Method
tb	536.28	K	Cheméo Relay (1.0)
tf	331.61	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C32118335&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point