

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.cheméo.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

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