

4-Bromo-2-methylphenyl isothiocyanate

Other names:	2-bromo-5-isothiocyanatotoluene
Inchi:	InChI=1S/C8H6BrNS/c1-6-4-7(9)2-3-8(6)10-5-11/h2-4H,1H3
InchiKey:	YASXCQRGYJGIKD-UHFFFAOYSA-N
Formula:	C8H6BrNS
SMILES:	<chem>Cc1cc(Br)ccc1N=C=S</chem>
Mol. weight [g/mol]:	228.11

Physical Properties

Property code	Value	Unit	Source
logp	3.492		Crippen Method
mcvol	135.050	ml/mol	McGowan Method
tb	512.90	K	Cheméo Relay (1.0)
tf	316.18	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C19241384&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):

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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<https://www.cheméo.com/cid/51-959-1/4-Bromo-2-methylphenyl-isothiocyanate.pdf>

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