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: Cc1cc(Br)ccc1N=C=S
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