

Benzene, 4-bromo-1-isothiocyanato-2-methyl-

Other names:	2-bromo-5-isothiocyanatoluene
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
CAS:	19241-38-4

Physical Properties

Property code	Value	Unit	Source
hf	315.54	kJ/mol	Joback Method
hvap	53.88	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.492		Crippen Method
mcvol	135.050	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	631.19	K	Joback Method
tc	906.91	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19241384&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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