

2-Bromothiophenol

Other names:	o-Bromothiophenol Benzenethiol, 2-bromo- o-Bromobenzenethiol Benzenethiol, o-bromo- 2-Bromobenzenethiol
Inchi:	InChI=1S/C6H5BrS/c7-5-3-1-2-4-6(5)8/h1-4,8H
InchiKey:	YUQUNWNSQDULTI-UHFFFAOYSA-N
Formula:	C6H5BrS
SMILES:	Sc1ccccc1Br
Mol. weight [g/mol]:	189.07
CAS:	6320-02-1

Physical Properties

Property code	Value	Unit	Source
gf	146.13	kJ/mol	Joback Method
hf	122.70	kJ/mol	Joback Method
hfus	14.28	kJ/mol	Joback Method
hvap	45.06	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.738		Crippen Method
mccvol	105.490	ml/mol	McGowan Method
pc	5527.84	kPa	Joback Method
tb	497.36	K	Joback Method
tc	761.63	K	Joback Method
tf	292.58	K	Joback Method
vc	0.380	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.21	J/mol×K	497.36	Joback Method
cpg	182.36	J/mol×K	541.40	Joback Method
cpg	190.75	J/mol×K	585.45	Joback Method
cpg	198.42	J/mol×K	629.49	Joback Method

cpg	205.42	J/mol×K	673.54	Joback Method
cpg	211.82	J/mol×K	717.58	Joback Method
cpg	217.66	J/mol×K	761.63	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.50 ± 1.50	K	0.80	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6320021&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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