

3-BROMOTHIOPHENOL

Other names:	Benzenethiol, 3-bromo- m-Bromothiophenol m-bromobenzenethiol
Inchi:	InChI=1S/C6H5BrS/c7-5-2-1-3-6(8)4-5/h1-4,8H
InchiKey:	HNGQQUDFJDROPY-UHFFFAOYSA-N
Formula:	C6H5BrS
SMILES:	Sc1cccc(Br)c1
Mol. weight [g/mol]:	189.08

Physical Properties

Property code	Value	Unit	Source
af	0.3211		Cheméo Relay (1.0)
gf	146.13	kJ/mol	Joback Method
hf	125.60	kJ/mol	Cheméo Relay (1.0)
hfus	14.28	kJ/mol	Joback Method
hvap	60.85	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
log10ws	-3.03		Cheméo Relay (1.0)
logp	2.738		Crippen Method
mcvol	105.490	ml/mol	McGowan Method
pc	5527.84	kPa	Joback Method
tb	504.50	K	Cheméo Relay (1.0)
tc	756.02	K	Cheméo Relay (1.0)
tf	269.38	K	Cheméo Relay (1.0)
vc	0.355	m3/kmol	Cheméo Relay (1.0)

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6320010&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):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tf:	Normal melting (fusion) point
vc:	Critical Volume

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