

Thiophene, 3-bromo-

Other names:	3-Bromothiophene 3-Thienyl bromide «beta»-Bromothiophene Â«betaÂ»-Bromothiophene
Inchi:	InChI=1S/C4H3BrS/c5-4-1-2-6-3-4/h1-3H
InchiKey:	XCMISAPCWHTVNG-UHFFFAOYSA-N
Formula:	C4H3BrS
SMILES:	Brc1ccsc1
Mol. weight [g/mol]:	163.04
CAS:	872-31-1

Physical Properties

Property code	Value	Unit	Source
ie	8.81	eV	NIST Webbook
ie	8.97	eV	NIST Webbook
ie	8.90 ± 0.05	eV	NIST Webbook
ie	9.02 ± 0.05	eV	NIST Webbook
ie	8.87	eV	NIST Webbook
ie	8.81 ± 0.01	eV	NIST Webbook
log10ws	-2.39		Crippen Method
logp	2.511		Crippen Method
mcvol	81.610	ml/mol	McGowan Method
rinpol	983.00		NIST Webbook
rinpol	983.00		NIST Webbook
tb	432.70	K	NIST Webbook
tb	423.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	28.90	kJ/mol	353.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.29748e+01
Coeff. B	-3.71689e+03
Coeff. C	1.21420e+01
Temperature range (K), min.	280.82
Temperature range (K), max.	472.88

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C872311&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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