

Thiophene, 2-bromo-

Other names:	2-Bromothiophene 2-Thienyl bromide Thienyl bromide
Inchi:	InChI=1S/C4H3BrS/c5-4-2-1-3-6-4/h1-3H
InchiKey:	TUCRZHGAIRVWTI-UHFFFAOYSA-N
Formula:	C4H3BrS
SMILES:	Brc1cccs1
Mol. weight [g/mol]:	163.04
CAS:	1003-09-4

Physical Properties

Property code	Value	Unit	Source
ie	8.60	eV	NIST Webbook
ie	8.66	eV	NIST Webbook
ie	8.93 ± 0.05	eV	NIST Webbook
ie	8.82 ± 0.05	eV	NIST Webbook
ie	8.63 ± 0.01	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.66 ± 0.01	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-2.39		Crippen Method
logp	2.511		Crippen Method
mvol	81.610	ml/mol	McGowan Method
rinpol	962.00		NIST Webbook
rinpol	962.00		NIST Webbook
sl	219.70	J/mol×K	NIST Webbook
tb	423.20	K	NIST Webbook
tf	203.90 ± 0.20	K	NIST Webbook
tt	204.30 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	144.00	J/mol×K	298.15	NIST Webbook

hfust	7.90	kJ/mol	203.90	NIST Webbook
hvapt	27.90	kJ/mol	353.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.29936e+01
Coeff. B	-3.68444e+03
Coeff. C	1.67700e+01
Temperature range (K), min.	273.21
Temperature range (K), max.	462.84

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1003094&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpl:	Liquid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
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
rinpola:	Non-polar retention indices
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature

tf: Normal melting (fusion) point

tt: Triple Point Temperature

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