

Benzene, 1-bromo-4-fluoro-

Other names:	1-Fluoro-4-bromobenzene
	1-bromo-4-fluorobenzene
	4-Bromo-1-fluorobenzene
	4-Bromofluorobenzene
	4-Fluoro-1-bromobenzene
	4-Fluorobromobenzene
	4-Fluorophenyl bromide
	NSC 10268
	p-Fluorobromobenzene
	p-Fluorophenyl bromide
	p-bromofluorobenzene
Inchi:	InChI=1S/C6H4BrF/c7-5-1-3-6(8)4-2-5/h1-4H
InchiKey:	AITNMTXHTIIBB-UHFFFAOYSA-N
Formula:	C6H4BrF
SMILES:	Fc1ccc(Br)cc1
Mol. weight [g/mol]:	175.00

Physical Properties

Property code	Value	Unit	Source
af	0.3061		Cheméo Relay (1.0)
gf	-78.07	kJ/mol	Joback Method
hf	-86.85	kJ/mol	Cheméo Relay (1.0)
hfus	13.31	kJ/mol	Joback Method
hvap	46.15	kJ/mol	Cheméo Relay (1.0)
ie	9.02 ± 0.02	eV	NIST Webbook
ie	8.99 ± 0.03	eV	NIST Webbook
ie	9.03	eV	NIST Webbook
log10ws	-2.73		Cheméo Relay (1.0)
logp	2.588		Crippen Method
mcvol	90.910	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
rinpol	896.90		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	940.90		NIST Webbook
tb	424.50 ± 0.50	K	NIST Webbook
tb	423.20	K	NIST Webbook

tc	643.64	K	Cheméo Relay (1.0)
tf	272.92	K	Cheméo Relay (1.0)
vc	0.331	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	144.15	J/mol×K	433.77	Joback Method
cpg	152.60	J/mol×K	471.11	Joback Method
cpg	160.46	J/mol×K	508.44	Joback Method
cpg	167.76	J/mol×K	545.78	Joback Method
cpg	174.52	J/mol×K	583.12	Joback Method
cpg	180.79	J/mol×K	620.45	Joback Method
cpg	186.59	J/mol×K	657.79	Joback Method
hvapt	44.00	kJ/mol	298.15	Vaporization enthalpies of a series of the halogen-substituted fluorobenzenes

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Vaporization enthalpies of a series of the halogen-substituted fluorobenzenes:	https://www.doi.org/10.1016/j.fluid.2014.12.023
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C460004&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

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
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
pc:	Critical Pressure
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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