

Benzene, 1-bromo-3-fluoro-

Other names:	1-Bromo-3-fluorobenzene 1-Fluoro-3-bromobenzene 3-Bromfluorbenzen 3-Bromofluorobenzene Benzene, 1-fluoro-3-bromo- NSC 10267 m-Bromofluorobenzene m-Fluorobromobenzene m-Fluorophenyl bromide
Inchi:	InChI=1S/C6H4BrF/c7-5-2-1-3-6(8)4-5/h1-4H
InchiKey:	QDFKKJYEIFBEFC-UHFFFAOYSA-N
Formula:	C6H4BrF
SMILES:	Fc1cccc(Br)c1
Mol. weight [g/mol]:	175.00
CAS:	1073-06-9

Physical Properties

Property code	Value	Unit	Source
gf	-78.07	kJ/mol	Joback Method
hf	-111.89	kJ/mol	Joback Method
hfus	13.31	kJ/mol	Joback Method
hvap	37.51	kJ/mol	Joback Method
ie	9.25	eV	NIST Webbook
ie	9.11 ± 0.02	eV	NIST Webbook
log10ws	-2.67		Aqueous Solubility Prediction Method
log10ws	-2.67		Estimated Solubility Method
logp	2.588		Crippen Method
mcvol	90.910	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
rinpol	932.80		NIST Webbook
tb	423.20	K	NIST Webbook
tb	423.00	K	NIST Webbook
tc	657.79	K	Joback Method
tf	256.71	K	Joback Method
vc	0.344	m ³ /kmol	Joback Method

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	44.30	kJ/mol	298.15	Vaporization enthalpies of a series of the halogen-substituted fluorobenzenes

Sources

Vaporization enthalpies of a series of the halogen-substituted fluorobenzenes:

<https://www.doi.org/10.1016/j.fluid.2014.12.023>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

Estimated Solubility Method:

http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1073069&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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