

2,4-Dibromo-1-fluorobenzene

Other names:	2,4-Dibromofluorobenzene 1-Fluoro-2,4-dibromobenzene Benzene, 2,4-dibromo-1-fluoro-
Inchi:	InChI=1S/C6H3Br2F/c7-4-1-2-6(9)5(8)3-4/h1-3H
InchiKey:	MKHDDTWHDFVYDQ-UHFFFAOYSA-N
Formula:	C6H3Br2F
SMILES:	Fc1ccc(Br)cc1Br
Mol. weight [g/mol]:	253.89
CAS:	1435-53-6

Physical Properties

Property code	Value	Unit	Source
gf	-73.38	kJ/mol	Joback Method
hf	-97.03	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	44.60	kJ/mol	Joback Method
ie	9.05 ± 0.02	eV	NIST Webbook
log10ws	-4.13		Crippen Method
logp	3.351		Crippen Method
mcvol	108.410	ml/mol	McGowan Method
pc	5102.04	kPa	Joback Method
tb	504.91	K	Joback Method
tc	748.62	K	Joback Method
tf	329.03	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.55	J/molxK	504.91	Joback Method
cpg	178.77	J/molxK	545.53	Joback Method
cpg	185.41	J/molxK	586.15	Joback Method
cpg	191.50	J/molxK	626.77	Joback Method
cpg	197.08	J/molxK	667.39	Joback Method

cpg	202.20	J/mol×K	708.00	Joback Method
cpg	206.91	J/mol×K	748.62	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.70	K	2.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1435536&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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