Benzene, bromopentafluoro-

Other names:	BROMOPERFLUOROBENZENE
	Bromopentafluorobenzene
	PENTAFLUOROPHENYL BROMIDE
	Pentafluorobromobenzene
Inchi:	InChI=1S/C6BrF5/c7-1-2(8)4(10)6(12)5(11)3(1)9
InchiKey:	XEKTVXADUPBFOA-UHFFFAOYSA-N
Formula:	C6BrF5
SMILES:	Fc1c(F)c(F)c(Br)c(F)c1F
Mol. weight [g/mol]:	246.96
CAS:	344-04-7

Physical Properties

Property code	Value	Unit	Source
af	0.3550		KDB
ea	1.15 ± 0.11	eV	NIST Webbook
gf	-895.83	kJ/mol	Joback Method
hf	-712.00 ± 5.60	kJ/mol	NIST Webbook
hfus	24.08	kJ/mol	Joback Method
hvap	43.05 ± 0.21	kJ/mol	NIST Webbook
hvap	43.10 ± 0.20	kJ/mol	NIST Webbook
ie	9.67 ± 0.02	eV	NIST Webbook
ie	9.60 ± 0.10	eV	NIST Webbook
ie	9.57	eV	NIST Webbook
ie	9.62 ± 0.05	eV	NIST Webbook
log10ws	-4.29		Crippen Method
logp	3.145		Crippen Method
mcvol	97.990	ml/mol	McGowan Method
pc	3000.00	kPa	KDB
tb	410.00	K	NIST Webbook
tb	410.00	K	NIST Webbook
tb	410.20	K	NIST Webbook
tb	410.00	K	NIST Webbook
tb	410.00	K	KDB
tc	601.00	K	KDB
tf	242.00	K	KDB
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.72	J/mol×K	450.77	Joback Method
cpg	182.89	J/mol×K	481.56	Joback Method
cpg	187.84	J/mol×K	512.35	Joback Method
cpg	192.57	J/mol×K	543.15	Joback Method
cpg	197.09	J/mol×K	573.94	Joback Method
cpg	201.39	J/mol×K	604.73	Joback Method
cpg	205.48	J/mol×K	635.52	Joback Method
hvapt	38.20	kJ/mol	461.00	NIST Webbook
hvapt	38.00	kJ/mol	468.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38810e+01
Coeff. B	-3.18029e+03
Coeff. C	-6.68050e+01
Temperature range (K), min.	300.76
Temperature range (K), max.	437.92

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.60422e+01
Coeff. B	-6.69908e+03
Coeff. C	-5.90024e+00
Coeff. D	2.47841e-06
Temperature range (K), min.	414.15
Temperature range (K), max.	521.15

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1660
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1660.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C344047&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume