

Benzene, 1,4-dibromo-2,3,5,6-tetrafluoro-

Other names:	Benzene, 1,4-dibromotetrafluoro- p-Dibromotetrafluorobenzene 1,4-Dibromo-2,3,5,6-tetrafluorobenzene 1,4-Dibromotetrafluorobenzene Tetrafluoro-1,4-dibromo benzene
Inchi:	InChI=1S/C6Br2F4/c7-1-3(9)5(11)2(8)6(12)4(1)10
InchiKey:	QFTZULJNRAHOIY-UHFFFAOYSA-N
Formula:	C6Br2F4
SMILES:	Fc1c(F)c(Br)c(F)c(F)c1Br
Mol. weight [g/mol]:	307.87
CAS:	344-03-6

Physical Properties

Property code	Value	Unit	Source
gf	-686.70	kJ/mol	Joback Method
hf	-719.77	kJ/mol	Joback Method
hfus	26.28	kJ/mol	Joback Method
hvap	44.14	kJ/mol	Joback Method
ie	9.42 ± 0.02	eV	NIST Webbook
log10ws	-5.12		Crippen Method
logp	3.768		Crippen Method
mcvol	113.720	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
tb	517.66	K	Joback Method
tc	728.35	K	Joback Method
tf	368.36	K	Joback Method
vc	0.460	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.65	J/mol×K	517.66	Joback Method
cpg	198.71	J/mol×K	552.78	Joback Method
cpg	203.47	J/mol×K	587.89	Joback Method

cpg	207.94	J/mol×K	623.01	Joback Method
cpg	212.14	J/mol×K	658.12	Joback Method
cpg	216.08	J/mol×K	693.24	Joback Method
cpg	219.77	J/mol×K	728.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C344036&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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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