

1-BROMO-2,3,4,6-TETRAFLUOROBENZENE

Other names:	2-bromo-1,3,4,5-tetrafluorobenzene Benzene, 2-bromo-1,3,4,5-tetrafluoro-
Inchi:	InChI=1S/C6HBrF4/c7-4-2(8)1-3(9)5(10)6(4)11/h1H
InchiKey:	AHJRONLVHNFUNH-UHFFFAOYSA-N
Formula:	C6HBrF4
SMILES:	Fc1cc(F)c(Br)c(F)c1F
Mol. weight [g/mol]:	228.97

Physical Properties

Property code	Value	Unit	Source
af	0.3793		Cheméo Relay (1.0)
hf	-557.26	kJ/mol	Cheméo Relay (1.0)
hfus	21.39	kJ/mol	Joback Method
hvap	46.50	kJ/mol	Cheméo Relay (1.0)
ie	9.40	eV	Cheméo Relay (1.0)
log10ws	-4.06		Cheméo Relay (1.0)
logp	3.006		Crippen Method
mcvol	96.220	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	420.92	K	Cheméo Relay (1.0)
tc	615.25	K	Cheméo Relay (1.0)
tf	235.62	K	Cheméo Relay (1.0)
vc	0.369	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.51	J/mol×K	446.52	Joback Method
cpg	175.39	J/mol×K	478.76	Joback Method
cpg	180.97	J/mol×K	511.01	Joback Method
cpg	186.26	J/mol×K	543.25	Joback Method
cpg	191.28	J/mol×K	575.49	Joback Method
cpg	196.03	J/mol×K	607.73	Joback Method
cpg	200.51	J/mol×K	639.98	Joback Method

Sources

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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1559860&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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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