1-BROMO-2,3,4,5-TETRAFLUOROBENZENE

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

Physical Properties

Property code	Value	Unit	Source
af	0.3824		Cheméo Relay (1.0)
hf	-544.99	kJ/mol	Cheméo Relay (1.0)
hfus	21.39	kJ/mol	Joback Method
hvap	46.67	kJ/mol	Cheméo Relay (1.0)
ie	9.44	eV	Cheméo Relay (1.0)
log10ws	-4.24		Cheméo Relay (1.0)
logp	3.006		Crippen Method
mcvol	96.220	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	416.10	K	Cheméo Relay (1.0)
tc	613.62	K	Cheméo Relay (1.0)
tf	244.94	K	Cheméo Relay (1.0)
vc	0.365	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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1074915&Units=SI
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):	

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