

1-Bromo-2,3,4,5-tetrachloro benzene

Inchi:	InChI=1S/C6HBrCl4/c7-2-1-3(8)5(10)6(11)4(2)9/h1H
InchiKey:	NEPMWYGBQGFJHN-UHFFFAOYSA-N
Formula:	C6HBrCl4
SMILES:	Clc1cc(Br)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	294.79
CAS:	1125-52-6

Physical Properties

Property code	Value	Unit	Source
gf	40.13	kJ/mol	Joback Method
hf	-13.15	kJ/mol	Joback Method
hfus	25.85	kJ/mol	Joback Method
hvap	57.85	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	5.063		Crippen Method
mcvol	138.100	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
tb	599.16	K	Joback Method
tc	860.80	K	Joback Method
tf	413.36	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.19	J/molxK	599.16	Joback Method
cpg	228.52	J/molxK	817.19	Joback Method
cpg	224.98	J/molxK	773.59	Joback Method
cpg	221.11	J/molxK	729.98	Joback Method
cpg	216.87	J/molxK	686.37	Joback Method
cpg	212.24	J/molxK	642.77	Joback Method
cpg	231.75	J/molxK	860.80	Joback Method
dvisc	0.0002864	Paxs	599.16	Joback Method
dvisc	0.0003335	Paxs	568.19	Joback Method

dvisc	0.0003952	Paxs	537.23	Joback Method
dvisc	0.0004782	Paxs	506.26	Joback Method
dvisc	0.0005932	Paxs	475.29	Joback Method
dvisc	0.0007582	Paxs	444.33	Joback Method
dvisc	0.0010054	Paxs	413.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1125526&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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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