

1,2,3,4-tetrabromobenzene

Inchi:	InChI=1S/C6H2Br4/c7-3-1-2-4(8)6(10)5(3)9/h1-2H
InchiKey:	QRFALSDGOMLVIR-UHFFFAOYSA-N
Formula:	C6H2Br4
SMILES:	BrC1ccc(Br)c(Br)c1Br
Mol. weight [g/mol]:	393.70
CAS:	22311-25-7

Physical Properties

Property code	Value	Unit	Source
gf	140.44	kJ/mol	Joback Method
hf	140.27	kJ/mol	Joback Method
hfus	25.31	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	4.737		Crippen Method
mcvol	141.640	ml/mol	McGowan Method
pc	6588.38	kPa	Joback Method
tb	642.94	K	Joback Method
tc	931.41	K	Joback Method
tf	460.56	K	Joback Method
vc	0.511	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.13	J/mol×K	642.94	Joback Method
cpg	212.32	J/mol×K	691.02	Joback Method
cpg	216.99	J/mol×K	739.10	Joback Method
cpg	221.24	J/mol×K	787.18	Joback Method
cpg	225.17	J/mol×K	835.26	Joback Method
cpg	228.87	J/mol×K	883.34	Joback Method
cpg	232.44	J/mol×K	931.41	Joback Method
dvisc	0.0008923	Paxs	460.56	Joback Method
dvisc	0.0006917	Paxs	490.96	Joback Method

dvisc	0.0005524	Paxs	521.35	Joback Method
dvisc	0.0004522	Paxs	551.75	Joback Method
dvisc	0.0003780	Paxs	582.15	Joback Method
dvisc	0.0003216	Paxs	612.54	Joback Method
dvisc	0.0002779	Paxs	642.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22311257&Units=SI
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

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
mccvol:	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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