Benzene, 1,2,4,5-tetrabromo-

Other names: 1,2,4,5-Tetrabromobenzene
2,3,5,6-Tetrabromobenzene
Inchi: InChI=1S/C6H2Br4/c7-3-1-4(8)6(10)2-5(3)9/h1-2H
InchiKey: QCKHVNQHBOGZER-UHFFFAOYSA-N
Formula: C6H2Br4
SMILES: Brc1cc(Br)c(Br)cc1Br
Mol. weight [g/mol]: 393.70
CAS: 636-28-2

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
ie	8.65	eV	NIST Webbook
ie	8.89	eV	NIST Webbook
log10ws	-6.98		Estimated Solubility Method
log10ws	-6.98		Aqueous Solubility Prediction 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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.87	J/mol×K	883.34	Joback Method
cpg	232.44	J/mol×K	931.41	Joback Method

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
dvisc	0.0003216	Pa×s	612.54	Joback Method
dvisc	0.0002779	Pa×s	642.94	Joback Method
dvisc	0.0008923	Pa×s	460.56	Joback Method
dvisc	0.0006917	Pa×s	490.96	Joback Method
dvisc	0.0005524	Pa×s	521.35	Joback Method
dvisc	0.0004522	Pa×s	551.75	Joback Method
dvisc	0.0003780	Pa×s	582.15	Joback Method
hfust	27.88	kJ/mol	453.10	NIST Webbook
hfust	0.34	kJ/mol	306.80	NIST Webbook
hfust	24.40	kJ/mol	454.50	NIST Webbook
hfust	27.88	kJ/mol	453.10	NIST Webbook
sfust	61.53	J/mol×K	453.10	NIST Webbook
sfust	1.09	J/mol×K	306.80	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C636282&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust: Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume