Benzene, 1,2,4-tribromo-

Other names: 1,2,4-Tribomobenzene
1,2,4-Tribromobenzene
Inchi: InChI=1S/C6H3Br3/c7-4-1-2-5(8)6(9)3-4/h1-3H
InchiKey: FWAJPSIPOULHHH-UHFFFAOYSA-N
Formula: C6H3Br3
SMILES: Brc1ccc(Br)c(Br)c1
Mol. weight [g/mol]: 314.80
CAS: 615-54-3

Physical Properties

Property code	Value	Unit	Source
gf	135.75	kJ/mol	Joback Method
hf	125.41	kJ/mol	Joback Method
hfus	20.41	kJ/mol	Joback Method
hvap	51.86	kJ/mol	Joback Method
log10ws	-4.50		Estimated Solubility Method
log10ws	-4.50		Aqueous Solubility Prediction Method
logp	3.974		Crippen Method
mcvol	124.140	ml/mol	McGowan Method
pc	6046.69	kPa	Joback Method
tb	548.20	K	NIST Webbook
tc	845.73	K	Joback Method
tf	316.32	K	Aqueous Solubility Prediction Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.07	J/mol×K	845.73	Joback Method
cpg	187.67	J/mol×K	571.80	Joback Method
cpg	194.29	J/mol×K	617.45	Joback Method
cpg	200.24	J/mol×K	663.11	Joback Method

cpg	205.62	J/mol×K	708.76	Joback Method
cpg	210.50	J/mol×K	754.42	Joback Method
cpg	214.96	J/mol×K	800.07	Joback Method
dvisc	0.0003256	Pa×s	571.80	Joback Method
dvisc	0.0012854	Pa×s	388.24	Joback Method
dvisc	0.0009405	Pa×s	418.83	Joback Method
dvisc	0.0007180	Pa×s	449.43	Joback Method
dvisc	0.0005674	Pa×s	480.02	Joback Method
dvisc	0.0004611	Pa×s	510.61	Joback Method
dvisc	0.0003837	Pa×s	541.21	Joback Method
hfust	17.90	kJ/mol	317.00	NIST Webbook

Sources

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=C615543&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
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