Benzene, 1,3,5-tribromo-

Other names:	1,3,5-Tribromobenzene
	Tribromobenzene
Inchi:	InChI=1S/C6H3Br3/c7-4-1-5(8)3-6(9)2-4/h1-3H
InchiKey:	YWDUZLFWHVQCHY-UHFFFAOYSA-N
Formula:	C6H3Br3
SMILES:	Brc1cc(Br)cc(Br)c1
Mol. weight [g/mol]:	314.80
CAS:	626-39-1

Physical Properties

Property code	Value	Unit	Source
gf	135.75	kJ/mol	Joback Method
hf	125.41	kJ/mol	Joback Method
hfus	21.72	kJ/mol	Low-Temperature Heat Capacities and Derived Thermodynamic Functions of 1,4 Dichlorobenzene, 1,4 Dibromobenzene, 1,3,5 Trichlorobenzene, and 1,3,5 Tribromobenzene
hvap	51.86	kJ/mol	Joback Method
ie	9.21 ± 0.02	eV	NIST Webbook
ie	8.91	eV	NIST Webbook
ie	9.21	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	-5.60		Estimated Solubility Method
log10ws	-5.60		Aqueous Solubility Prediction Method
logp	3.974		Crippen Method
mcvol	124.140	ml/mol	McGowan Method
pc	6046.69	kPa	Joback Method
tb	544.20	K	NIST Webbook
tc	845.73	K	Joback Method
tf	396.42	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	21.72	kJ/mol	395.00	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C626391&Units=SI

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

Low-Temperature Heat Capacities and Derived Thermodynamic Functions of 1,4 Dichlorobenzene, 1,4 Dibromobenzene, 1,3,5 Trichlorobenzene, and 1,3,5 Tribromobenzene: https://www.doi.org/10.1021/je049762q

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume