

1,2,3-TRIBROMOBENZENE

Inchi:	InChI=1S/C6H3Br3/c7-4-2-1-3-5(8)6(4)9/h1-3H
InchiKey:	GMVJKSNPLYBFSO-UHFFFAOYSA-N
Formula:	C6H3Br3
SMILES:	BrC1CCCC(Br)c1Br
Mol. weight [g/mol]:	314.80

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	-5.05		Aqueous Solubility Prediction Method
logp	3.974		Crippen Method
mcvol	124.140	ml/mol	McGowan Method
pc	6046.69	kPa	Joback Method
tb	571.80	K	Joback Method
tc	845.73	K	Joback Method
tf	360.65	K	Aqueous Solubility Prediction Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.67	J/molxK	571.80	Joback Method
cpg	214.96	J/molxK	800.07	Joback Method
cpg	210.50	J/molxK	754.42	Joback Method
cpg	205.62	J/molxK	708.76	Joback Method
cpg	200.24	J/molxK	663.11	Joback Method
cpg	194.29	J/molxK	617.45	Joback Method
cpg	219.07	J/molxK	845.73	Joback Method
dvisc	0.0003256	Paxs	571.80	Joback Method

dvisc	0.0003837	Paxs	541.21	Joback Method
dvisc	0.0004611	Paxs	510.61	Joback Method
dvisc	0.0005674	Paxs	480.02	Joback Method
dvisc	0.0007180	Paxs	449.43	Joback Method
dvisc	0.0009405	Paxs	418.83	Joback Method
dvisc	0.0012854	Paxs	388.24	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

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
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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