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/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
cpg	219.07	J/mol×K	845.73	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
dvisc	0.0003256	Pa×s	571.80	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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