Phenol, pentabromo-

Other names:	2,3,4,5,6-pentabromophenol
	Flammex 5BP
	Pentabromfenol
	pentabromophenol
Inchi:	InChI=1S/C6HBr5O/c7-1-2(8)4(10)6(12)5(11)3(1)9/h12H
InchiKey:	SVHOVVJFOWGYJO-UHFFFAOYSA-N
Formula:	C6HBr5O
SMILES:	Oc1c(Br)c(Br)c(Br)c(Br)c1Br
Mol. weight [g/mol]:	488.59
CAS:	608-71-9

Physical Properties

Property code	Value	Unit	Source
gf	-9.49	kJ/mol	Joback Method
hf	-22.18	kJ/mol	Joback Method
hfus	35.99	kJ/mol	Joback Method
hvap	79.06	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.205		Crippen Method
mcvol	165.010	ml/mol	McGowan Method
pc	9444.29	kPa	Joback Method
tb	794.70	K	Joback Method
tc	1099.10	K	Joback Method
tf	644.60	K	Joback Method
tt	416.20	K	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.14	J/mol×K	794.70	Joback Method

cpg	251.87	J/mol×K	845.43	Joback Method
cpg	255.89	J/mol×K	896.17	Joback Method
cpg	260.42	J/mol×K	946.90	Joback Method
cpg	265.69	J/mol×K	997.63	Joback Method
cpg	271.93	J/mol×K	1048.36	Joback Method
cpg	279.37	J/mol×K	1099.10	Joback Method
dvisc	0.0000136	Pa×s	794.70	Joback Method
dvisc	0.0000406	Pa×s	669.62	Joback Method
dvisc	0.0000316	Pa×s	694.63	Joback Method
dvisc	0.0000531	Pa×s	644.60	Joback Method
dvisc	0.0000202	Pa×s	744.67	Joback Method
dvisc	0.0000165	Pa×s	769.68	Joback Method
dvisc	0.0000251	Pa×s	719.65	Joback Method
hfust	27.60	kJ/mol	469.80	NIST Webbook
hfust	19.14	kJ/mol	502.00	NIST Webbook
hfust	11.29	kJ/mol	441.50	NIST Webbook
hfust	19.14	kJ/mol	502.00	NIST Webbook
sfust	25.57	J/mol×K	441.50	NIST Webbook
sfust	38.13	J/mol×K	502.00	NIST Webbook

Sources

Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants:	https://www.doi.org/10.1021/acs.jced.7b01040
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C608719&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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