Phenol, 2,4,6-tribromo-

Other names:	Bromkal Pur 3
	Bromol
	Flammex 3BP
	2,4,6-Tribromophenol
	TA 10
	Emery 9332
	FR-613
	Great Lakes PH-73
	1,3,5-Tribromo-2-hydroxybenzene
	NSC 2136
	TBP
	PH 73
Inchi:	InChI=1S/C6H3Br3O/c7-3-1-4(8)6(10)5(9)2-3/h1-2,10H
InchiKey:	BSWWXRFVMJHFBN-UHFFFAOYSA-N
Formula:	C6H3Br3O
SMILES:	Oc1c(Br)cc(Br)cc1Br
Mol. weight [g/mol]:	330.80
CAS:	118-79-6

Physical Properties

Property code	Value	Unit	Source
chs	-2689.20 ± 3.50	kJ/mol	NIST Webbook
gf	-18.87	kJ/mol	Joback Method
hf	-0.90 ± 2.50	kJ/mol	NIST Webbook
hfs	-98.50 ± 2.30	kJ/mol	NIST Webbook
hfs	-101.00 ± 4.00	kJ/mol	NIST Webbook
hfus	26.20	kJ/mol	Joback Method
hsub	97.60 ± 1.10	kJ/mol	NIST Webbook
hvap	64.87	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.680		Crippen Method
mcvol	130.010	ml/mol	McGowan Method
pc	7735.33	kPa	Joback Method
rinpol	1576.00		NIST Webbook
rinpol	278.50		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1624.00		NIST Webbook

tb	652.42	K	Joback Method
tc	934.99	K	Joback Method
tf	366.00 ± 3.00	K	NIST Webbook
tf	368.00 ± 1.50	K	NIST Webbook
tf	368.65 ± 2.00	K	NIST Webbook
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.05	J/mol×K	887.90	Joback Method
cpg	237.59	J/mol×K	840.80	Joback Method
cpg	246.73	J/mol×K	934.99	Joback Method
cpg	218.69	J/mol×K	652.42	Joback Method
cpg	223.92	J/mol×K	699.52	Joback Method
cpg	228.70	J/mol×K	746.61	Joback Method
cpg	233.20	J/mol×K	793.71	Joback Method
cps	172.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0000376	Pa×s	652.42	Joback Method
dvisc	0.0000646	Pa×s	601.60	Joback Method
dvisc	0.0000488	Pa×s	627.01	Joback Method
dvisc	0.0002647	Pa×s	499.96	Joback Method
dvisc	0.0001768	Pa×s	525.37	Joback Method
dvisc	0.0001225	Pa×s	550.78	Joback Method
dvisc	0.0000877	Pa×s	576.19	Joback Method
hfust	18.52	kJ/mol	366.20	NIST Webbook
hfust	18.52	kJ/mol	366.20	NIST Webbook
hfust	20.90	kJ/mol	367.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	559.20	K	99.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C118796&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume