Phenol, 2,6-dibromo-

Other names: 2,6-Dibromophenol
Inchi: InChI=1S/C6H4Br2O/c7-4-2-1-3-5(8)6(4)9/h1-3,9H
InchiKey: SSIZLKDLDKIHEV-UHFFFAOYSA-N
Formula: C6H4Br2O
SMILES: Oc1c(Br)cccc1Br
Mol. weight [g/mol]: 251.90
CAS: 608-33-3

Physical Properties

Property code	Value	Unit	Source
gf	-23.56	kJ/mol	Joback Method
hf	-66.76	kJ/mol	Joback Method
hfus	83.40	kJ/mol	Thermochemical study of three dibromophenol isomers
hvap	57.77	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.917		Crippen Method
mcvol	112.510	ml/mol	McGowan Method
pc	7049.79	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1333.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2370.00		NIST Webbook
ripol	2365.00		NIST Webbook
tb	581.28	K	Joback Method
tc	849.80	K	Joback Method
tf	427.64	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	199.13	J/mol×K	581.28	Joback Method
cpg	205.80	J/mol×K	626.03	Joback Method
cpg	211.78	J/mol×K	670.79	Joback Method
cpg	217.20	J/mol×K	715.54	Joback Method
cpg	222.21	J/mol×K	760.29	Joback Method
cpg	226.94	J/mol×K	805.05	Joback Method
cpg	231.54	J/mol×K	849.80	Joback Method
dvisc	0.0007319	Pa×s	427.64	Joback Method
dvisc	0.0004349	Pa×s	453.25	Joback Method
dvisc	0.0002732	Pa×s	478.85	Joback Method
dvisc	0.0001800	Pa×s	504.46	Joback Method
dvisc	0.0001234	Pa×s	530.07	Joback Method
dvisc	0.0000876	Pa×s	555.67	Joback Method
dvisc	0.0000641	Pa×s	581.28	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	528.70	K	98.70	NIST Webbook

Sources

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Thermochemical study of three dibromophenol isomers: https://www.doi.org/10.1016/j.jct.2010.08.020

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=C608333&Units=SI

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
rinpol:	Non-polar retention indices
ripol:	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

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