

Phenol, 2,4-dibromo-

Other names:	2,4-dibromophenol DBP Emery 9331 FR-612
Inchi:	InChI=1S/C6H4Br2O/c7-4-1-2-6(9)5(8)3-4/h1-3,9H
InchiKey:	FAXWFCTVSHEODL-UHFFFAOYSA-N
Formula:	C6H4Br2O
SMILES:	Oc1ccc(Br)cc1Br
Mol. weight [g/mol]:	251.90
CAS:	615-58-7

Physical Properties

Property code	Value	Unit	Source
gf	-23.56	kJ/mol	Joback Method
hf	-66.76	kJ/mol	Joback Method
hfus	81.30	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
tb	581.28	K	Joback Method
tc	849.80	K	Joback Method
tf	427.64	K	Joback Method
vc	0.353	m ³ /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/molxK	715.54	Joback Method
cpg	222.21	J/molxK	760.29	Joback Method
cpg	226.94	J/molxK	805.05	Joback Method
cpg	231.54	J/molxK	849.80	Joback Method
dvisc	0.0007319	Paxs	427.64	Joback Method
dvisc	0.0004349	Paxs	453.25	Joback Method
dvisc	0.0002732	Paxs	478.85	Joback Method
dvisc	0.0001800	Paxs	504.46	Joback Method
dvisc	0.0001234	Paxs	530.07	Joback Method
dvisc	0.0000876	Paxs	555.67	Joback Method
dvisc	0.0000641	Paxs	581.28	Joback Method

Sources

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=C615587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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