3,5-dibromophenol

Inchi: InChI=1S/C6H4Br2O/c7-4-1-5(8)3-6(9)2-4/h1-3,9H
InchiKey: PZFMWYNHJFZBPO-UHFFFAOYSA-N
Formula: C6H4Br2O
SMILES: Oc1cc(Br)cc(Br)c1
Mol. weight [g/mol]: 251.91

Physical Properties

Property code	Value	Unit	Source
gf	-23.56	kJ/mol	Joback Method
hf	-66.76	kJ/mol	Joback Method
hfus	94.30	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.54	J/mol×K	849.80	Joback Method
cpg	205.80	J/mol×K	626.03	Joback Method
cpg	211.78	J/mol×K	670.79	Joback Method
cpg	222.21	J/mol×K	760.29	Joback Method
cpg	226.94	J/mol×K	805.05	Joback Method
cpg	217.20	J/mol×K	715.54	Joback Method
cpg	199.13	J/mol×K	581.28	Joback Method
dvisc	0.0007319	Pa×s	427.64	Joback Method

dvisc	0.0002732	Pa×s	478.85	Joback Method
dvisc	0.0001800	Pa×s	504.46	Joback Method
dvisc	0.0000641	Pa×s	581.28	Joback Method
dvisc	0.0001234	Pa×s	530.07	Joback Method
dvisc	0.0000876	Pa×s	555.67	Joback Method
dvisc	0.0004349	Pa×s	453.25	Joback Method
psub	6.29e-04	kPa	313.19	Thermochemical study of three dibromophenol isomers
psub	4.07e-04	kPa	309.11	Thermochemical study of three dibromophenol isomers
psub	4.14e-04	kPa	309.11	Thermochemical study of three dibromophenol isomers
psub	3.89e-04	kPa	309.11	Thermochemical study of three dibromophenol isomers
psub	5.02e-04	kPa	311.13	Thermochemical study of three dibromophenol isomers
psub	5.01e-04	kPa	311.13	Thermochemical study of three dibromophenol isomers
psub	4.93e-04	kPa	311.13	Thermochemical study of three dibromophenol isomers
psub	6.63e-04	kPa	313.19	Thermochemical study of three dibromophenol isomers
psub	3.17e-04	kPa	307.18	Thermochemical study of three dibromophenol isomers
psub	6.50e-04	kPa	313.19	Thermochemical study of three dibromophenol isomers
psub	8.13e-04	kPa	315.21	Thermochemical study of three dibromophenol isomers
psub	8.38e-04	kPa	315.21	Thermochemical study of three dibromophenol isomers

psub	8.01e-04	kPa	315.21	Thermochemical study of three dibromophenol isomers
psub	1.01e-03	kPa	317.12	Thermochemical study of three dibromophenol isomers
psub	1.02e-03	kPa	317.12	Thermochemical study of three dibromophenol isomers
psub	9.93e-04	kPa	317.12	Thermochemical study of three dibromophenol isomers
psub	3.15e-04	kPa	307.18	Thermochemical study of three dibromophenol isomers
psub	3.25e-04	kPa	307.18	Thermochemical study of three dibromophenol isomers
psub	2.42e-04	kPa	305.11	Thermochemical study of three dibromophenol isomers
psub	2.44e-04	kPa	305.11	Thermochemical study of three dibromophenol isomers
psub	2.41e-04	kPa	305.11	Thermochemical study of three dibromophenol isomers
psub	1.89e-04	kPa	303.20	Thermochemical study of three dibromophenol isomers
psub	1.84e-04	kPa	303.20	Thermochemical study of three dibromophenol isomers
psub	1.96e-04	kPa	303.20	Thermochemical study of three dibromophenol isomers
psub	1.51e-04	kPa	301.19	Thermochemical study of three dibromophenol isomers
psub	1.46e-04	kPa	301.19	Thermochemical study of three dibromophenol isomers
psub	1.57e-04	kPa	301.19	Thermochemical study of three dibromophenol isomers

psub	1.17e-04	kPa	299.19	Thermochemical study of three dibromophenol isomers
psub	1.18e-04	kPa	299.19	Thermochemical study of three dibromophenol isomers
psub	1.20e-04	kPa	299.19	Thermochemical study of three dibromophenol isomers

Sources

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
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
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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume