3,5-Dibromosalicylaldehyde

Other names:	3,5-Dibromo-2-hydroxybenzaldehyde Benzaldehyde, 3,5-dibromo-2-hydroxy- Dalyde Salicylaldehyde, 3,5-dibromo- 2-Hydroxy-3,5-dibromobenzaldehyde 3,5-Dibromosalicylaldeyde
Inchi:	InChI=1S/C7H4Br2O2/c8-5-1-4(3-10)7(11)6(9)2-5/h1-3,11H
InchiKey:	JHZOXYGFQMROFJ-UHFFFAOYSA-N
Formula:	C7H4Br2O2
SMILES:	O=Cc1cc(Br)cc(Br)c1O
Mol. weight [g/mol]:	279.91
CAS:	90-59-5

Physical Properties

Property code	Value	Unit	Source
gf	-124.29	kJ/mol	Joback Method
hf	-184.45	kJ/mol	Joback Method
hfus	25.79	kJ/mol	Joback Method
hvap	67.38	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	2.730		Crippen Method
mcvol	128.170	ml/mol	McGowan Method
pc	6631.37	kPa	Joback Method
tb	657.80	K	Joback Method
tc	921.09	K	Joback Method
tf	493.43	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.67	J/mol×K	657.80	Joback Method
cpg	251.83	J/mol×K	701.68	Joback Method
cpg	257.50	J/mol×K	745.56	Joback Method

cpg	262.81	J/mol×K	789.45	Joback Method
cpg	267.88	J/mol×K	833.33	Joback Method
cpg	272.84	J/mol×K	877.21	Joback Method
cpg	277.82	J/mol×K	921.09	Joback Method
dvisc	0.0003476	Pa×s	493.43	Joback Method
dvisc	0.0002227	Pa×s	520.82	Joback Method
dvisc	0.0001492	Pa×s	548.22	Joback Method
dvisc	0.0001038	Pa×s	575.62	Joback Method
dvisc	0.0000747	Pa×s	603.01	Joback Method
dvisc	0.0000553	Pa×s	630.40	Joback Method
dvisc	0.0000420	Pa×s	657.80	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C90595&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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