5,6-Dibromovanillin

Other names: 2,3-Dibromo-4-hydroxy-5-methoxybenzaldehyde
Inchi: InChI=1S/C8H6Br2O3/c1-13-5-2-4(3-11)6(9)7(10)8(5)12/h2-3,12H,1H3
InchiKey: WKLKGSHBXNPUDU-UHFFFAOYSA-N
Formula: C8H6Br2O3
SMILES: COc1cc(C=O)c(Br)c(Br)c1O
Mol. weight [g/mol]: 309.94
CAS: 2973-75-3

Physical Properties

Property code	Value	Unit	Source
gf	-230.50	kJ/mol	Joback Method
hf	-348.78	kJ/mol	Joback Method
hfus	29.18	kJ/mol	Joback Method
hvap	72.68	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	2.738		Crippen Method
mcvol	148.130	ml/mol	McGowan Method
pc	5438.52	kPa	Joback Method
tb	708.08	K	Joback Method
tc	961.42	K	Joback Method
tf	539.45	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.89	J/mol×K	708.08	Joback Method
cpg	317.18	J/mol×K	750.30	Joback Method
cpg	324.03	J/mol×K	792.53	Joback Method
cpg	330.54	J/mol×K	834.75	Joback Method
cpg	336.79	J/mol×K	876.98	Joback Method
cpg	342.86	J/mol×K	919.20	Joback Method
cpg	348.82	J/mol×K	961.42	Joback Method
dvisc	0.0001554	Pa×s	539.45	Joback Method

dvisc	0.0001043	Pa×s	567.56	Joback Method
dvisc	0.0000727	Pa×s	595.66	Joback Method
dvisc	0.0000524	Pa×s	623.76	Joback Method
dvisc	0.0000388	Pa×s	651.87	Joback Method
dvisc	0.0000295	Pa×s	679.97	Joback Method
dvisc	0.0000229	Pa×s	708.08	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=C2973753&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