2,5-Dibromobenzoic acid

Other names: benzoic acid, 2,5-dibromo-
Inchi: InChI=1S/C7H4Br2O2/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,(H,10,11)
InchiKey: SQQKOTVDGCJJKI-UHFFFAOYSA-N
Formula: C7H4Br2O2
SMILES: O=C(O)c1cc(Br)ccc1Br
Mol. weight [g/mol]: 279.91
CAS: 610-71-9

Physical Properties

Property code	Value	Unit	Source
gf	-135.89	kJ/mol	Joback Method
hf	-186.37	kJ/mol	Joback Method
hfus	23.41	kJ/mol	Joback Method
hvap	71.07	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	2.910		Crippen Method
mcvol	128.170	ml/mol	McGowan Method
pc	5953.74	kPa	Joback Method
tb	674.57	K	Joback Method
tc	911.01	K	Joback Method
tf	428.15 ± 1.00	K	NIST Webbook
tf	428.00	K	Vapor pressures, standard molar enthalpies, entropies Gibbs energies of sublimation and heat capacities of 2,5- and 3,5-dibromobenzoic acids
tf	425.65 ± 1.00	K	NIST Webbook
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.39	J/mol×K	674.57	Joback Method
cpg	249.49	J/mol×K	713.98	Joback Method

cpg	255.10	J/mol×K	753.38	Joback Method
cpg	260.26	J/mol×K	792.79	Joback Method
cpg	265.01	J/mol×K	832.20	Joback Method
cpg	269.40	J/mol×K	871.60	Joback Method
cpg	273.46	J/mol×K	911.01	Joback Method
dvisc	0.0011214	Pa×s	450.46	Joback Method
dvisc	0.0006253	Pa×s	487.81	Joback Method
dvisc	0.0003789	Pa×s	525.16	Joback Method
dvisc	0.0002454	Pa×s	562.51	Joback Method
dvisc	0.0001678	Pa×s	599.87	Joback Method
dvisc	0.0001199	Pa×s	637.22	Joback Method
dvisc	0.0000890	Pa×s	674.57	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor pressures, standard molar enthalpies, entropies Gibbs energies of sublimation and heat capacities of 2,5- and 3,5-dibromobenzoic acids:	https://www.doi.org/10.1016/j.fluid.2012.11.006
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=C610719&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