Phenol, 2,4-dibromo-, acetate

Other names: Acetic acid, 2,4-dibromophenyl ester
Inchi: InChI=1S/C8H6Br2O2/c1-5(11)12-8-3-2-6(9)4-7(8)10/h2-4H,1H3
InchiKey: RXBCSBQMWRLETO-UHFFFAOYSA-N
Formula: C8H6Br2O2
SMILES: CC(=O)Oc1ccc(Br)cc1Br
Mol. weight [g/mol]: 293.94
CAS: 36914-79-1

Physical Properties

Property code	Value	Unit	Source
gf	-95.65	kJ/mol	Joback Method
hf	-187.00	kJ/mol	Joback Method
hfus	23.10	kJ/mol	Joback Method
hvap	59.03	kJ/mol	Joback Method
ie	8.21 ± 0.03	eV	NIST Webbook
log10ws	-4.11		Crippen Method
logp	3.137		Crippen Method
mcvol	142.260	ml/mol	McGowan Method
pc	4438.52	kPa	Joback Method
tb	627.69	K	Joback Method
tc	878.22	K	Joback Method
tf	423.14	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.61	J/mol×K	627.69	Joback Method
cpg	283.58	J/mol×K	669.45	Joback Method
cpg	291.87	J/mol×K	711.20	Joback Method
cpg	299.53	J/mol×K	752.96	Joback Method
cpg	306.56	J/mol×K	794.71	Joback Method
cpg	313.01	J/mol×K	836.47	Joback Method
cpg	318.89	J/mol×K	878.22	Joback Method

dvisc	0.0010566	Pa×s	423.14	Joback Method
dvisc	0.0007517	Pa×s	457.23	Joback Method
dvisc	0.0005606	Pa×s	491.32	Joback Method
dvisc	0.0004344	Pa×s	525.41	Joback Method
dvisc	0.0003472	Pa×s	559.51	Joback Method
dvisc	0.0002847	Pa×s	593.60	Joback Method
dvisc	0.0002385	Pa×s	627.69	Joback Method

Sources

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=C36914791&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
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