perbenzoic acid

Inchi: InChI=1S/C7H6O3/c8-7(10-9)6-4-2-1-3-5-6/h1-5,9H
InchiKey: XCRBXWCUXJNEFX-UHFFFAOYSA-N
Formula: C7H6O3
SMILES: O=C(OO)c1ccccc1
Mol. weight [g/mol]: 138.12
CAS: 93-59-4

Physical Properties

Property code	Value	Unit	Source
gf	-250.27	kJ/mol	Joback Method
hf	-348.31	kJ/mol	Joback Method
hfs	-367.00 ± 13.00	kJ/mol	NIST Webbook
hfus	14.80	kJ/mol	Joback Method
hvap	59.29	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.316		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	4952.36	kPa	Joback Method
tb	554.71	K	Joback Method
tc	762.15	K	Joback Method
tf	328.05	K	Joback Method
vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.80	J/mol×K	554.71	Joback Method
cpg	223.27	J/mol×K	589.28	Joback Method
cpg	231.24	J/mol×K	623.86	Joback Method
cpg	238.70	J/mol×K	658.43	Joback Method
cpg	245.69	J/mol×K	693.00	Joback Method
cpg	252.19	J/mol×K	727.58	Joback Method
cpg	258.24	J/mol×K	762.15	Joback Method
dvisc	0.0052845	Pa×s	328.05	Joback Method

dvisc	0.0019974	Pa×s	365.83	Joback Method
dvisc	0.0009058	Pa×s	403.60	Joback Method
dvisc	0.0004703	Pa×s	441.38	Joback Method
dvisc	0.0002708	Pa×s	479.16	Joback Method
dvisc	0.0001690	Pa×s	516.93	Joback Method
dvisc	0.0001125	Pa×s	554.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93594&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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