1,4-Benzenediol, monobenzoate

Other names: 1,4-Diphenol, 1-benzoate
p-hydroxyphenyl benzoate
Inchi: InChI=1S/C13H10O3/c14-11-6-8-12(9-7-11)16-13(15)10-4-2-1-3-5-10/h1-9,14H
InchiKey: JFAXJRJMFOACBO-UHFFFAOYSA-N
Formula: C13H10O3
SMILES: O=C(Oc1ccc(O)cc1)c1ccccc1
Mol. weight [g/mol]: 214.22
CAS: 2444-19-1

Physical Properties

Property code	Value	Unit	Source
gf	-105.14	kJ/mol	Joback Method
hf	-260.70	kJ/mol	Joback Method
hfus	26.08	kJ/mol	Joback Method
hvap	71.25	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.611		Crippen Method
mcvol	159.820	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
tb	707.11	K	Joback Method
tc	962.79	K	Joback Method
tf	472.99	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.44	J/mol×K	707.11	Joback Method
cpg	467.02	J/mol×K	920.18	Joback Method
cpg	457.84	J/mol×K	877.56	Joback Method
cpg	448.02	J/mol×K	834.95	Joback Method
cpg	437.42	J/mol×K	792.34	Joback Method
cpg	425.94	J/mol×K	749.72	Joback Method
cpg	475.68	J/mol×K	962.79	Joback Method

dvisc	0.0000147	Pa×s	707.11	Joback Method
dvisc	0.0000213	Pa×s	668.09	Joback Method
dvisc	0.0000323	Pa×s	629.07	Joback Method
dvisc	0.0000517	Pa×s	590.05	Joback Method
dvisc	0.0000885	Pa×s	551.03	Joback Method
dvisc	0.0001645	Pa×s	512.01	Joback Method
dvisc	0.0003388	Pa×s	472.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2444191&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
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