

1,4-Benzenedicarboxylic acid, 2,3-dihydroxy-

Other names:	2,3-Dihydroxyterephthalic acid
Inchi:	InChI=1S/C8H6O6/c9-5-3(7(11)12)1-2-4(6(5)10)8(13)14/h1-2,9-10H,(H,11,12)(H,13,14)
InchiKey:	OHLSHRJUBRUKAN-UHFFFAOYSA-N
Formula:	C8H6O6
SMILES:	O=C(O)c1ccc(C(=O)O)c(O)c1O
Mol. weight [g/mol]:	198.13
CAS:	19829-72-2

Physical Properties

Property code	Value	Unit	Source
gf	-721.46	kJ/mol	Joback Method
hf	-867.63	kJ/mol	Joback Method
hfus	33.07	kJ/mol	Joback Method
hvap	109.22	kJ/mol	Joback Method
log10ws	-0.69		Crippen Method
logp	0.494		Crippen Method
mcvol	126.440	ml/mol	McGowan Method
pc	8866.47	kPa	Joback Method
tb	867.44	K	Joback Method
tc	1086.85	K	Joback Method
tf	663.80	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.55	J/mol×K	867.44	Joback Method
cpg	354.44	J/mol×K	904.01	Joback Method
cpg	360.44	J/mol×K	940.58	Joback Method
cpg	366.66	J/mol×K	977.15	Joback Method
cpg	373.21	J/mol×K	1013.72	Joback Method
cpg	380.18	J/mol×K	1050.29	Joback Method
cpg	387.69	J/mol×K	1086.85	Joback Method
dvisc	0.0000008	Pa×s	663.80	Joback Method

dvisc	0.0000004	Pa×s	697.74	Joback Method
dvisc	0.0000002	Pa×s	731.68	Joback Method
dvisc	0.0000001	Pa×s	765.62	Joback Method
dvisc	6.1733088e-08	Pa×s	799.56	Joback Method
dvisc	3.7091542e-08	Pa×s	833.50	Joback Method
dvisc	2.3192351e-08	Pa×s	867.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19829722&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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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