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

Physical Properties

Property code	Value	Unit	Source
hf	-1024.38	kJ/mol	Cheméo Relay (1.0)
hfus	33.07	kJ/mol	Joback Method
ie	9.03	eV	Cheméo Relay (1.0)
log10ws	-1.65		Cheméo Relay (1.0)
logp	0.494		Crippen Method
mcvol	126.440	ml/mol	McGowan Method
tb	560.46	K	Cheméo Relay (1.0)
tc	949.51	K	Cheméo Relay (1.0)
tf	502.97	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.55	J/mol×K	867.44	Joback Method
cpg	387.69	J/mol×K	1086.85	Joback Method
cpg	380.18	J/mol×K	1050.29	Joback Method
cpg	373.21	J/mol×K	1013.72	Joback Method
cpg	366.66	J/mol×K	977.15	Joback Method
cpg	360.44	J/mol×K	940.58	Joback Method
cpg	354.44	J/mol×K	904.01	Joback Method
dvisc	0.0000001	Pa×s	765.62	Joback Method
dvisc	2.3192351e-08	Pa×s	867.44	Joback Method
dvisc	3.7091542e-08	Pa×s	833.50	Joback Method
dvisc	6.1733088e-08	Pa×s	799.56	Joback Method
dvisc	0.0000008	Pa×s	663.80	Joback Method

dvisc	0.0000002	Pa×s	731.68	Joback Method
dvisc	0.0000004	Pa×s	697.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19829722&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point