Benzoic acid, 2,4-dihydroxy-6-methyl-

Other names:	«beta»-Resorcylic acid, 6-methyl-
	o-Orsellinic acid
	Orcinolcarboxylic acid
	Orsellic acid
	Orsellinic acid
	2,4-Dihydroxy-6-methylbenzenecarboxylic acid
	2,4-Dihydroxy-6-methylbenzoic acid
	4,6-Dihydroxy-o-toluic acid
	4,6-Dihydroxy-2-methylbenzoic acid
	6-Methyl-«beta»-resorcylic acid
Inchi:	InChI=1S/C8H8O4/c1-4-2-5(9)3-6(10)7(4)8(11)12/h2-3,9-10H,1H3,(H,11,12)
InchiKey:	AMKYESDOVDKZKV-UHFFFAOYSA-N
Formula:	C8H8O4
SMILES:	Cc1cc(O)cc(O)c1C(=O)O
Mol. weight [g/mol]:	168.15
CAS:	480-64-8

Physical Properties

Property code	Value	Unit	Source
gf	-455.72	kJ/mol	Joback Method
hf	-602.82	kJ/mol	Joback Method
hfus	27.38	kJ/mol	Joback Method
hvap	85.79	kJ/mol	Joback Method
log10ws	-1.10		Crippen Method
logp	1.104		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	6751.79	kPa	Joback Method
rinpol	1745.00		NIST Webbook
rinpol	1745.00		NIST Webbook
tb	721.39	K	Joback Method
tc	947.05	K	Joback Method
tf	553.05	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.00	J/mol×K	721.39	Joback Method
cpg	320.01	J/mol×K	759.00	Joback Method
cpg	326.73	J/mol×K	796.61	Joback Method
cpg	333.29	J/mol×K	834.22	Joback Method
cpg	339.78	J/mol×K	871.83	Joback Method
cpg	346.34	J/mol×K	909.44	Joback Method
cpg	353.06	J/mol×K	947.05	Joback Method
dvisc	0.0000158	Pa×s	553.05	Joback Method
dvisc	0.0000078	Pa×s	581.11	Joback Method
dvisc	0.0000041	Pa×s	609.16	Joback Method
dvisc	0.0000023	Pa×s	637.22	Joback Method
dvisc	0.0000014	Pa×s	665.28	Joback Method
dvisc	0.0000008	Pa×s	693.33	Joback Method
dvisc	0.0000005	Pa×s	721.39	Joback Method

Sources

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=C480648&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume