1,3-Benzenediol, 4,5-dimethyl-

Other names:	Resorcinol, 4,5-dimethyl-
	o-Xylorcinol
	1,2-Dimethyl-3,5-dihydroxybenzene
	1,3-Dihydroxy-4,5-dimethylbenzene
	3,5-Dihydroxy-1,2-dimethylbenzene
	4,5-Dimethylresorcinol
Inchi:	InChI=1S/C8H10O2/c1-5-3-7(9)4-8(10)6(5)2/h3-4,9-10H,1-2H3
InchiKey:	RCNCKKACINZDOI-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	Cc1cc(O)cc(O)c1C
Mol. weight [g/mol]:	138.16
CAS:	527-55-9

Physical Properties

Property code	Value	Unit	Source
gf	-189.98	kJ/mol	Joback Method
hf	-338.01	kJ/mol	Joback Method
hfus	21.69	kJ/mol	Joback Method
hvap	62.37	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.715		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	5312.41	kPa	Joback Method
tb	575.34	K	Joback Method
tc	814.79	K	Joback Method
tf	442.30	K	Joback Method
vc	0.307	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.75	J/mol×K	814.79	Joback Method
cpg	312.26	J/mol×K	774.89	Joback Method
cpg	304.55	J/mol×K	734.98	Joback Method

cpg	296.46	J/mol×K	695.07	Joback Method
cpg	287.88	J/mol×K	655.16	Joback Method
cpg	278.66	J/mol×K	615.25	Joback Method
cpg	268.68	J/mol×K	575.34	Joback Method
dvisc	0.0002320	Pa×s	442.30	Joback Method
dvisc	0.0000097	Pa×s	575.34	Joback Method
dvisc	0.0000148	Pa×s	553.17	Joback Method
dvisc	0.0000234	Pa×s	530.99	Joback Method
dvisc	0.0000386	Pa×s	508.82	Joback Method
dvisc	0.0000664	Pa×s	486.65	Joback Method
dvisc	0.0001205	Pa×s	464.47	Joback Method
hvapt	67.50	kJ/mol	438.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C527559&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

hvapt: Enthalpy of vaporization at a given temperature

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