

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:	<chem>Cc1cc(O)cc(O)c1C</chem>
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.68	J/mol×K	575.34	Joback Method
cpg	278.66	J/mol×K	615.25	Joback Method
cpg	287.88	J/mol×K	655.16	Joback Method

cpg	296.46	J/mol×K	695.07	Joback Method
cpg	304.55	J/mol×K	734.98	Joback Method
cpg	312.26	J/mol×K	774.89	Joback Method
cpg	319.75	J/mol×K	814.79	Joback Method
dvisc	0.0002320	Paxs	442.30	Joback Method
dvisc	0.0001205	Paxs	464.47	Joback Method
dvisc	0.0000664	Paxs	486.65	Joback Method
dvisc	0.0000386	Paxs	508.82	Joback Method
dvisc	0.0000234	Paxs	530.99	Joback Method
dvisc	0.0000148	Paxs	553.17	Joback Method
dvisc	0.0000097	Paxs	575.34	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

Latest version available from:

<https://www.cheméo.com/cid/88-279-6/1-3-Benzenediol-4-5-dimethyl.pdf>

Generated by Cheméo on 2025-12-05 13:29:23.35545358 +0000 UTC m=+4689560.885494245.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.