1,4-Benzenediol, 2,3,5-trimethyl-

Other names:	«psi»-Cumohydroquinone
	Hydroquinone, trimethyl-
	Pseudocumohydroquinone
	2,3,5-Trimethyl-1,4-benzenediol
	Trimethylhydroquinone
	2,3,5-Trimethylhydroquinone
	psi-Cumohydroquinone
	2,3,6-Trimethylhydroquinone
	NSC 401617
Inchi:	InChI=1S/C9H12O2/c1-5-4-8(10)6(2)7(3)9(5)11/h4,10-11H,1-3H3
InchiKey:	AUFZRCJENRSRLY-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	Cc1cc(O)c(C)c(C)c1O
Mol. weight [g/mol]:	152.19
CAS:	700-13-0

Physical Properties

Property code	Value	Unit	Source
gf	-191.19	kJ/mol	Joback Method
hf	-370.12	kJ/mol	Joback Method
hfus	23.89	kJ/mol	Joback Method
hvap	65.26	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	2.023		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	4546.92	kPa	Joback Method
tb	603.20	K	Joback Method
tc	838.77	K	Joback Method
tf	443.15 ± 0.70	K	NIST Webbook
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	360.12	J/mol×K	799.51	Joback Method
cpg	312.30	J/mol×K	603.20	Joback Method
cpg	323.00	J/mol×K	642.46	Joback Method
cpg	333.01	J/mol×K	681.72	Joback Method
cpg	342.46	J/mol×K	720.98	Joback Method
cpg	351.45	J/mol×K	760.25	Joback Method
cpg	368.59	J/mol×K	838.77	Joback Method
cpl	217.60	J/mol×K	313.65	NIST Webbook
dvisc	0.0000063	Pa×s	603.20	Joback Method
dvisc	0.0001252	Pa×s	466.09	Joback Method
dvisc	0.0000678	Pa×s	488.94	Joback Method
dvisc	0.0000388	Pa×s	511.79	Joback Method
dvisc	0.0000233	Pa×s	534.64	Joback Method
dvisc	0.0000146	Pa×s	557.50	Joback Method
dvisc	0.0000095	Pa×s	580.35	Joback Method
hvapt	45.50 ± 0.30	kJ/mol	475.50	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C700130&Units=SI

Legend

cpg: Ideal gas heat capacity
cpl: Liquid phase 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