1,2-Benzenediol, 3-methyl-

Other names:	1,2-Dihydroxy-3-methylbenzene
	2,3-Dihydroxytoluene
	2,3-Toluenediol
	2-Hydroxy-3-methylphenol
	3-Methyl-1,2-benzenediol
	3-Methyl-1,2-benzenediol (3-methylpyrocatechol)
	3-Methyl-1,2-dihydroxybenzene
	3-Methylcatechol
	3-Methylpyrocatechol
	Catechol, 3-methyl-
	NSC 66523
	Pyrocatechol, 3-methyl-
Inchi:	InChI=1S/C7H8O2/c1-5-3-2-4-6(8)7(5)9/h2-4,8-9H,1H3
InchiKey:	PGSWEKYNAOWQDF-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	Cc1cccc(O)c1O
Mol. weight [g/mol]:	124.14
CAS:	488-17-5

Physical Properties

Property code	Value	Unit	Source
chs	-3505.40 ± 0.50	kJ/mol	NIST Webbook
gf	-188.77	kJ/mol	Joback Method
hf	-299.30 ± 1.60	kJ/mol	NIST Webbook
hfs	-392.50 ± 1.10	kJ/mol	NIST Webbook
hfus	19.49	kJ/mol	Joback Method
hsub	93.20 ± 1.00	kJ/mol	NIST Webbook
hsub	93.20 ± 1.00	kJ/mol	NIST Webbook
hsub	93.20	kJ/mol	NIST Webbook
hvap	59.48	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	1.406		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
pc	6288.83	kPa	Joback Method
rinpol	1263.00		NIST Webbook
rinpol	1263.00		NIST Webbook
ripol	2627.00		NIST Webbook

ripol	2627.00		NIST Webbook
tb	514.20	K	NIST Webbook
tc	790.85	K	Joback Method
tf	418.51	K	Joback Method
vc	0.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.69	J/mol×K	547.48	Joback Method
cpg	265.88	J/mol×K	750.29	Joback Method
cpg	259.16	J/mol×K	709.73	Joback Method
cpg	252.03	J/mol×K	669.16	Joback Method
cpg	244.34	J/mol×K	628.60	Joback Method
cpg	235.94	J/mol×K	588.04	Joback Method
cpg	272.32	J/mol×K	790.85	Joback Method
dvisc	0.0000153	Pa×s	547.48	Joback Method
dvisc	0.0000240	Pa×s	525.99	Joback Method
dvisc	0.0000392	Pa×s	504.49	Joback Method
dvisc	0.0000667	Pa×s	483.00	Joback Method
dvisc	0.0001192	Pa×s	461.50	Joback Method
dvisc	0.0002256	Pa×s	440.00	Joback Method
dvisc	0.0004561	Pa×s	418.51	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	3.96155e+01
Coeff. B	-1.16997e+04
Coeff. C	-1.29762e+02
Temperature range (K), min.	427.25
Temperature range (K), max.	470.82

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=C488175&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume