1,2-Benzenediol, 3-methoxy-

Other names:	Pyrocatechol, 3-methoxy-
	Pyrogallol 1-methyl ether
	Pyrogallol 1-monomethyl ether
	1,2-Dihydroxy-3-methoxybenzene
	2,3-Dihydroxyanisole
	3-Methoxy-1,2-benzenediol
	3-Methoxycatechol
	3-Methoxypyrocatechol
	1-O-Methylpyrogallol
	3-Methoxy-o-hydroquinone
	6-Methoxycatechol
	NSC 66525
	3-Methoxy-1,2-benzenediol (3-methoxypyrocatechol)
Inchi:	InChI=1S/C7H8O3/c1-10-6-4-2-3-5(8)7(6)9/h2-4,8-9H,1H3
InchiKey:	LPYUENQFPVNPHY-UHFFFAOYSA-N
Formula:	C7H8O3
SMILES:	COc1cccc(O)c1O
Mol. weight [g/mol]:	140.14
CAS:	934-00-9

Physical Properties

Property code	Value	Unit	Source
chs	-3387.70 ± 0.70	kJ/mol	NIST Webbook
gf	-293.77	kJ/mol	Joback Method
hf	-418.50 ± 1.40	kJ/mol	NIST Webbook
hfs	-510.20 ± 1.20	kJ/mol	NIST Webbook
hfus	20.68	kJ/mol	Joback Method
hsub	91.70 ± 0.80	kJ/mol	NIST Webbook
hsub	91.70	kJ/mol	NIST Webbook
hvap	91.70 ± 0.80	kJ/mol	NIST Webbook
log10ws	-0.69		Crippen Method
logp	1.106		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
pc	6122.63	kPa	Joback Method
rinpol	1272.00		NIST Webbook
rinpol	1268.20		NIST Webbook
rinpol	1269.80		NIST Webbook

tb	569.90	K	Joback Method
tc	809.70	K	Joback Method
tf	440.74	K	Joback Method
vc	0.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.31	J/mol×K	569.90	Joback Method
cpg	256.37	J/mol×K	609.87	Joback Method
cpg	264.71	J/mol×K	649.83	Joback Method
cpg	272.46	J/mol×K	689.80	Joback Method
cpg	279.72	J/mol×K	729.77	Joback Method
cpg	286.62	J/mol×K	769.73	Joback Method
cpg	293.27	J/mol×K	809.70	Joback Method
dvisc	0.0002233	Pa×s	440.74	Joback Method
dvisc	0.0001166	Pa×s	462.27	Joback Method
dvisc	0.0000645	Pa×s	483.79	Joback Method
dvisc	0.0000375	Pa×s	505.32	Joback Method
dvisc	0.0000228	Pa×s	526.85	Joback Method
dvisc	0.0000144	Pa×s	548.37	Joback Method
dvisc	0.0000094	Pa×s	569.90	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	419.70	K	2.00	NIST Webbook
tbrp	402.20	K	1.30	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

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