1,3-Benzodioxol-5-ol

Other names:	Phenol, 3,4-(methylenedioxy)-
	Sesamol
	3,4-(Methylenedioxy)phenol
	5-Hydroxy-1,3-benzodioxole
	Methylene ether of oxyhydroquinone
	5-Hydroxy-1,3-benzodioxole (sesamol)
Inchi:	InChI=1S/C7H6O3/c8-5-1-2-6-7(3-5)10-4-9-6/h1-3,8H,4H2
InchiKey:	LUSZGTFNYDARNI-UHFFFAOYSA-N
Formula:	C7H6O3
SMILES:	Oc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	138.12
CAS:	533-31-3

Physical Properties

Property code	Value	Unit	Source
gf	-147.56	kJ/mol	Joback Method
hf	-310.92	kJ/mol	Joback Method
hfus	26.34	kJ/mol	Joback Method
hsub	92.20 ± 0.60	kJ/mol	NIST Webbook
hvap	56.37	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.121		Crippen Method
mcvol	92.480	ml/mol	McGowan Method
pc	6103.52	kPa	Joback Method
rinpol	1278.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1312.00		NIST Webbook
tb	537.15	K	Joback Method
tc	782.79	K	Joback Method
tf	394.63	K	Joback Method
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.64	J/mol×K	782.79	Joback Method
cpg	217.31	J/mol×K	537.15	Joback Method
cpg	226.75	J/mol×K	578.09	Joback Method
cpg	235.27	J/mol×K	619.03	Joback Method
cpg	242.99	J/mol×K	659.97	Joback Method
cpg	250.04	J/mol×K	700.91	Joback Method
cpg	256.55	J/mol×K	741.85	Joback Method
dvisc	0.0001410	Pa×s	537.15	Joback Method
dvisc	0.0016410	Pa×s	394.63	Joback Method
dvisc	0.0009706	Pa×s	418.38	Joback Method
dvisc	0.0006074	Pa×s	442.14	Joback Method
dvisc	0.0003987	Pa×s	465.89	Joback Method
dvisc	0.0002727	Pa×s	489.64	Joback Method
dvisc	0.0001931	Pa×s	513.40	Joback Method
hfust	16.96	kJ/mol	337.70	NIST Webbook
hsubt	92.10 ± 0.60	kJ/mol	301.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C533313&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

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
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume