1,4-dimethoxybenzene

Other names: Benzene, 1,4-dimethoxy-
Inchi: InChI=1S/C8H10O2/c1-9-7-3-5-8(10-2)6-4-7/h3-6H,1-2H3
InchiKey: OHBQPCCCRFSCAX-UHFFFAOYSA-N
Formula: C8H10O2
SMILES: COc1ccc(OC)cc1
Mol. weight [g/mol]: 138.16
CAS: 150-78-7

Physical Properties

Property code	Value	Unit	Source
gf	-90.74	kJ/mol	Joback Method
hf	-247.83	kJ/mol	Joback Method
hfus	12.50	kJ/mol	Joback Method
hsub	84.10 ± 2.30	kJ/mol	NIST Webbook
hvap	41.16	kJ/mol	Joback Method
ie	7.90	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	7.53 ± 0.03	eV	NIST Webbook
ie	7.54	eV	NIST Webbook
ie	7.90 ± 0.10	eV	NIST Webbook
ie	7.83 ± 0.01	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	7.96	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	7.70 ± 0.15	eV	NIST Webbook
ie	7.45	eV	NIST Webbook
ie	7.78 ± 0.03	eV	NIST Webbook
ie	7.56 ± 0.11	eV	NIST Webbook
log10ws	-1.71		Crippen Method
logp	1.704		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
rinpol	1185.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1145.00		NIST Webbook

rinpol	1145.00		NIST Webbook
rinpol	1180.10		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1143.40		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1143.40		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1165.21		NIST Webbook
rinpol	1167.74		NIST Webbook
rinpol	1180.10		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1171.00		NIST Webbook
ripol	1752.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1759.00		NIST Webbook
ripol	1727.00		NIST Webbook
ripol	1728.00		NIST Webbook
ripol	1757.00		NIST Webbook
ripol	1747.00		NIST Webbook
tb	485.80 ± 1.50	K	NIST Webbook
tb	485.80	K	NIST Webbook
tc	667.35	K	Joback Method
tf	329.45 ± 0.60	K	NIST Webbook
tf	329.00 ± 3.00	K	NIST Webbook
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.28	J/mol×K	458.94	Joback Method
cpg	232.94	J/mol×K	493.67	Joback Method
cpg	244.14	J/mol×K	528.41	Joback Method
cpg	254.88	J/mol×K	563.14	Joback Method
cpg	265.14	J/mol×K	597.88	Joback Method
cpg	274.92	J/mol×K	632.61	Joback Method
cpg	284.22	J/mol×K	667.35	Joback Method
dvisc	0.0014041	Pa×s	263.32	Joback Method
dvisc	0.0008184	Pa×s	295.92	Joback Method
dvisc	0.0005310	Pa×s	328.53	Joback Method
dvisc	0.0003725	Pa×s	361.13	Joback Method
dvisc	0.0002771	Pa×s	393.73	Joback Method
dvisc	0.0002157	Pa×s	426.34	Joback Method
dvisc	0.0001740	Pa×s	458.94	Joback Method
hvapt	62.10	kJ/mol	327.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.20	K	2.70	NIST Webbook

Sources

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=C150787&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
ripol:	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