1,3-dimethoxybenzene

Other names: Benzene, 1,3-dimethoxy-
Inchi: InChI=1S/C8H10O2/c1-9-7-4-3-5-8(6-7)10-2/h3-6H,1-2H3
InchiKey: DPZNOMCNRMUKPS-UHFFFAOYSA-N
Formula: C8H10O2
SMILES: COc1cccc(OC)c1
Mol. weight [g/mol]: 138.16
CAS: 151-10-0

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
hvap	61.50 ± 1.40	kJ/mol	NIST Webbook
ie	8.18	eV	NIST Webbook
ie	8.14	eV	NIST Webbook
ie	8.00 ± 0.15	eV	NIST Webbook
ie	8.20 ± 0.10	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	1175.00		NIST Webbook
rinpol	1138.80		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1138.80		NIST Webbook
rinpol	1181.90		NIST Webbook
rinpol	1147.00		NIST Webbook
ripol	1737.00		NIST Webbook
ripol	1740.00		NIST Webbook
ripol	1761.00		NIST Webbook
ripol	1730.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1709.00		NIST Webbook

ripol	1730.00		NIST Webbook
tb	490.25 ± 1.00	K	NIST Webbook
tb	490.70	K	NIST Webbook
tc	667.35	K	Joback Method
tf	237.85 ± 0.30	K	NIST Webbook
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.22	J/mol×K	667.35	Joback Method
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
dvisc	0.0001740	Pa×s	458.94	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
hvapt	60.80	kJ/mol	390.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.20	K	0.90	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=C151100&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
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