

2,4-Dimethoxyiodobenzene

Other names:	1,3-Dimethoxy-4-iodobenzene Benzene, 1-iodo-2,4-dimethoxy-
Inchi:	InChI=1S/C8H9IO2/c1-10-6-3-4-7(9)8(5-6)11-2/h3-5H,1-2H3
InchiKey:	ZDUYJCKEORTAQE-UHFFFAOYSA-N
Formula:	C8H9IO2
SMILES:	COc1ccc(I)c(OC)c1
Mol. weight [g/mol]:	264.06
CAS:	20469-63-0

Physical Properties

Property code	Value	Unit	Source
gf	-42.25	kJ/mol	Joback Method
hf	-182.43	kJ/mol	Joback Method
hfus	16.52	kJ/mol	Joback Method
hvap	51.19	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.308		Crippen Method
mcvol	137.380	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
tb	557.06	K	Joback Method
tc	799.44	K	Joback Method
tf	333.90	K	Joback Method
vc	0.499	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.74	J/molxK	557.06	Joback Method
cpg	315.11	J/molxK	759.04	Joback Method
cpg	306.47	J/molxK	718.65	Joback Method
cpg	297.20	J/molxK	678.25	Joback Method
cpg	287.32	J/molxK	637.85	Joback Method
cpg	276.83	J/molxK	597.46	Joback Method
cpg	323.14	J/molxK	799.44	Joback Method

dvisc	0.0001901	Paxs	557.06	Joback Method
dvisc	0.0002333	Paxs	519.87	Joback Method
dvisc	0.0002955	Paxs	482.67	Joback Method
dvisc	0.0003893	Paxs	445.48	Joback Method
dvisc	0.0005393	Paxs	408.29	Joback Method
dvisc	0.0007977	Paxs	371.09	Joback Method
dvisc	0.0012872	Paxs	333.90	Joback Method

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=C20469630&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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