4-Iododiphenyl ether

Other names:	Benzene, 1,1'-oxybis(4-iodo-
	Bis(p-iodophenyl) ether
	Ether, bis(p-iodophenyl)
	4-Iododiphenyl ether
	4,4'-Diiododiphenyl ether
Inchi:	InChI=1S/C12H9IO/c13-10-6-8-12(9-7-10)14-11-4-2-1-3-5-11/h1-9H
InchiKey:	BDKOUDYNKRCDEC-UHFFFAOYSA-N
Formula:	C12H9IO
SMILES:	Ic1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	296.11

Physical Properties

Property code	Value	Unit	Source
af	0.4568		Cheméo Relay (1.0)
gf	218.47	kJ/mol	Joback Method
hf	131.26	kJ/mol	Cheméo Relay (1.0)
hfus	20.12	kJ/mol	Joback Method
hvap	78.03	kJ/mol	Cheméo Relay (1.0)
ie	7.76	eV	Cheméo Relay (1.0)
log10ws	-5.48		Cheméo Relay (1.0)
logp	4.083		Crippen Method
mcvol	164.110	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
tb	603.03	K	Cheméo Relay (1.0)
tc	868.03	K	Cheméo Relay (1.0)
tf	314.99	K	Cheméo Relay (1.0)
vc	0.568	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.42	J/mol×K	647.86	Joback Method
cpg	363.19	J/mol×K	694.20	Joback Method
cpg	375.68	J/mol×K	740.54	Joback Method

cpg	386.97	J/mol×K	786.88	Joback Method
cpg	397.16	J/mol×K	833.22	Joback Method
cpg	406.33	J/mol×K	879.56	Joback Method
cpg	414.57	J/mol×K	925.90	Joback Method
dvisc	0.0015233	Pa×s	370.65	Joback Method
dvisc	0.0008544	Pa×s	416.85	Joback Method
dvisc	0.0005379	Pa×s	463.05	Joback Method
dvisc	0.0003683	Pa×s	509.25	Joback Method
dvisc	0.0002686	Pa×s	555.46	Joback Method
dvisc	0.0002056	Pa×s	601.66	Joback Method
dvisc	0.0001635	Pa×s	647.86	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28896493&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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