4-Iodoanisole

Other names:	1-iodo-4-methoxybenzene
	4-Iodomethoxybenzene
	4-Methoxy-1-iodobenzene
	4-Methoxyiodobenzene
	4-Methoxyphenyl iodide
	Anisole, p-iodo-
	Isoform
	NSC 60727
	anisole, 4-iodo-
	benzene, 1-iodo-4-methoxy-
	p-Iodoanisol
	p-Iodomethoxybenzene
	p-Iodophenyl methyl ether
	p-Methoxyiodobenzene
	p-Methoxyphenyl iodide
	p-iodoanisole
Inchi:	InChI=1S/C7H7IO/c1-9-7-4-2-6(8)3-5-7/h2-5H,1H3
InchiKey:	SYSZENVIJHPFNL-UHFFFAOYSA-N
Formula:	C7H7IO
SMILES:	COc1ccc(I)cc1
Mol. weight [g/mol]:	234.04
CAS:	696-62-8

Physical Properties

Property code	Value	Unit	Source
hf	16.41	kJ/mol	Cheméo Relay (1.0)
hfus	13.13	kJ/mol	Joback Method
hvap	53.10 ± 0.40	kJ/mol	NIST Webbook
ie	7.97	eV	NIST Webbook
log10ws	-3.66		Cheméo Relay (1.0)
logp	2.300		Crippen Method
mcvol	117.420	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
rinpol	1326.00		NIST Webbook
rinpol	1326.00		NIST Webbook
ripol	1852.00		NIST Webbook
tb	524.79	K	Cheméo Relay (1.0)

tc	746.58	K	Cheméo Relay (1.0)
tf	312.10	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.29	J/mol×K	506.78	Joback Method
cpg	213.57	J/mol×K	548.42	Joback Method
cpg	223.17	J/mol×K	590.05	Joback Method
cpg	232.11	J/mol×K	631.69	Joback Method
cpg	240.42	J/mol×K	673.33	Joback Method
cpg	248.13	J/mol×K	714.96	Joback Method
cpg	255.25	J/mol×K	756.60	Joback Method
dvisc	0.0022544	Pa×s	287.88	Joback Method
dvisc	0.0012898	Pa×s	324.36	Joback Method
dvisc	0.0008261	Pa×s	360.85	Joback Method
dvisc	0.0005743	Pa×s	397.33	Joback Method
dvisc	0.0004244	Pa×s	433.81	Joback Method
dvisc	0.0003286	Pa×s	470.30	Joback Method
dvisc	0.0002641	Pa×s	506.78	Joback Method
hvapt	83.40	kJ/mol	298.15	Experimental and computational study of the molecular energetics of the monoiodoanisole isomers
hvapt	54.40	kJ/mol	460.50	NIST Webbook
hvapt	53.10 ± 0.40	kJ/mol	440.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	510.20	K	96.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49989e+01
Coeff. B	-4.61300e+03
Coeff. C	-6.67600e+01
Temperature range (K), min.	380.33
Temperature range (K), max.	542.95

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0, beta):	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Experimental and computational study of the molecular energetics of the	https://www.doi.org/10.1016/j.jct.2011.12.001
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C696628&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
pvap:	Vapor 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