2-Iodoanisole

Other names:	1-iodo-2-methoxybenzene
	Anisole, o-iodo-
	Benzene, 1-iodo-2-methoxy-
	Iodanisol
	o-Anisyl iodide
	o-Iodoanisole
Inchi:	InChI=1S/C7H7IO/c1-9-7-5-3-2-4-6(7)8/h2-5H,1H3
InchiKey:	DVQWNQBEUKXONL-UHFFFAOYSA-N
Formula:	C7H7IO
SMILES:	COc1ccccc1I
Mol. weight [g/mol]:	234.03
CAS:	529-28-2

Physical Properties

Property code	Value	Unit	Source
gf	63.96	kJ/mol	Joback Method
hf	-18.10	kJ/mol	Joback Method
hfus	13.13	kJ/mol	Joback Method
hvap	45.90	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.300		Crippen Method
mcvol	117.420	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
rinpol	1268.40		NIST Webbook
tb	506.78	K	Joback Method
tc	756.60	K	Joback Method
tf	287.88	K	Joback Method
vc	0.425	m3/kmol	Joback Method

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	65.30	kJ/mol	298.15	Experimental and computational study of the molecular energetics of the monoiodoanisole isomers

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.70	K	2.50	NIST Webbook
tbrp	512.70	K	97.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C529282&Units=SI

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

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

Experimental and computational study of the molecular energetics of the monoiodoanisole isomers: https://www.doi.org/10.1016/j.jct.2011.12.001

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume