Methyl-2-iodobenzoate

Other names:	Benzoic acid, 2-iodo-, methyl ester
	Benzoic acid, o-iodo-, methyl ester
	Methyl o-iodobenzoate
	2-Iodobenzoic acid methyl ester
	o-Iodobenzoic acid, methyl ester
Inchi:	InChI=1S/C8H7IO2/c1-11-8(10)6-4-2-3-5-7(6)9/h2-5H,1H3
InchiKey:	BXXLTVBTDZXPTN-UHFFFAOYSA-N
Formula:	C8H7IO2
SMILES:	COC(=O)c1ccccc1I
Mol. weight [g/mol]:	262.04
CAS:	610-97-9

Physical Properties

Property code	Value	Unit	Source
chl	-3905.30 ± 4.20	kJ/mol	NIST Webbook
gf	-56.54	kJ/mol	Joback Method
hf	-151.32	kJ/mol	Joback Method
hfus	17.32	kJ/mol	Joback Method
hvap	54.87	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.078		Crippen Method
mcvol	133.080	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1439.00		NIST Webbook
rinpol	1439.00		NIST Webbook
tb	583.53	K	Joback Method
tc	836.60	K	Joback Method
tf	349.08	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	255.67	J/mol×K	583.53	Joback Method
cpg	265.96	J/mol×K	625.71	Joback Method
cpg	275.50	J/mol×K	667.89	Joback Method
cpg	284.30	J/mol×K	710.06	Joback Method
cpg	292.40	J/mol×K	752.24	Joback Method
cpg	299.81	J/mol×K	794.42	Joback Method
cpg	306.58	J/mol×K	836.60	Joback Method
dvisc	0.0019750	Pa×s	349.08	Joback Method
dvisc	0.0011856	Pa×s	388.16	Joback Method
dvisc	0.0007813	Pa×s	427.23	Joback Method
dvisc	0.0005522	Pa×s	466.31	Joback Method
dvisc	0.0004118	Pa×s	505.38	Joback Method
dvisc	0.0003203	Pa×s	544.45	Joback Method
dvisc	0.0002576	Pa×s	583.53	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=C610979&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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