1-Iodo-3,4-methylenedioxybenzene

Inchi: InChI=1S/C7H5IO2/c8-5-1-2-6-7(3-5)10-4-9-6/h1-3H,4H2
InchiKey: NMMCBIXYIYQHCP-UHFFFAOYSA-N
Formula: C7H5IO2
SMILES: Ic1ccc2c(c1)OCO2
Mol. weight [g/mol]: 248.02
CAS: 5876-51-7

Physical Properties

Property code	Value	Unit	Source
gf	55.55	kJ/mol	Joback Method
hf	-68.21	kJ/mol	Joback Method
hfus	24.58	kJ/mol	Joback Method
hvap	53.39	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.020		Crippen Method
mcvol	112.430	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
tb	554.65	K	Joback Method
tc	823.57	K	Joback Method
tf	353.49	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.55	J/mol×K	554.65	Joback Method
cpg	251.59	J/mol×K	778.75	Joback Method
cpg	245.39	J/mol×K	733.93	Joback Method
cpg	238.59	J/mol×K	689.11	Joback Method
cpg	231.08	J/mol×K	644.29	Joback Method
cpg	222.78	J/mol×K	599.47	Joback Method
cpg	257.31	J/mol×K	823.57	Joback Method
dvisc	0.0006189	Pa×s	554.65	Joback Method
dvisc	0.0007315	Pa×s	521.12	Joback Method

dvisc	0.0008847	Pa×s	487.60	Joback Method
dvisc	0.0011006	Pa×s	454.07	Joback Method
dvisc	0.0014175	Pa×s	420.54	Joback Method
dvisc	0.0019076	Pa×s	387.02	Joback Method
dvisc	0.0027158	Pa×s	353.49	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C5876517&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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