(3-Iodophenyl) methanol, isopropyl ether

Inchi: InChI=1S/C10H13IO/c1-8(2)12-7-9-4-3-5-10(11)6-9/h3-6,8H,7H2,1-2H3
InchiKey: OVVXNPIIRXUEEI-UHFFFAOYSA-N
Formula: C10H13IO
SMILES: CC(C)OCc1cccc(I)c1
Mol. weight [g/mol]: 276.11

Physical Properties

Property code	Value	Unit	Source
gf	86.78	kJ/mol	Joback Method
hf	-85.30	kJ/mol	Joback Method
hfus	17.38	kJ/mol	Joback Method
hvap	52.19	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.216		Crippen Method
mcvol	159.690	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
rinpol	1507.00		NIST Webbook
tb	574.98	K	Joback Method
tc	815.29	K	Joback Method
tf	306.69	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.32	J/mol×K	574.98	Joback Method
cpg	348.37	J/mol×K	615.03	Joback Method
cpg	361.51	J/mol×K	655.08	Joback Method
cpg	373.77	J/mol×K	695.13	Joback Method
cpg	385.17	J/mol×K	735.18	Joback Method
cpg	395.77	J/mol×K	775.23	Joback Method
cpg	405.59	J/mol×K	815.29	Joback Method
dvisc	0.0026835	Pa×s	306.69	Joback Method
dvisc	0.0012986	Pa×s	351.40	Joback Method

dvisc	0.0007403	Pa×s	396.12	Joback Method
dvisc	0.0004730	Pa×s	440.84	Joback Method
dvisc	0.0003282	Pa×s	485.55	Joback Method
dvisc	0.0002422	Pa×s	530.26	Joback Method
dvisc	0.0001874	Pa×s	574.98	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=U374572&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume