(3-Iodophenyl) methanol, 2-methylpropyl ether

Inchi: InChI=1S/C11H15IO/c1-9(2)7-13-8-10-4-3-5-11(12)6-10/h3-6,9H,7-8H2,1-2H3
InchiKey: DQXCQDONIAOAGW-UHFFFAOYSA-N
Formula: C11H15IO
SMILES: CC(C)COCc1cccc(I)c1
Mol. weight [g/mol]: 290.14

Physical Properties

Property code	Value	Unit	Source
gf	95.20	kJ/mol	Joback Method
hf	-105.94	kJ/mol	Joback Method
hfus	19.97	kJ/mol	Joback Method
hvap	54.41	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.464		Crippen Method
mcvol	173.780	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1602.00		NIST Webbook
tb	597.86	K	Joback Method
tc	833.23	K	Joback Method
tf	317.96	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.45	J/mol×K	597.86	Joback Method
cpg	396.33	J/mol×K	637.09	Joback Method
cpg	410.26	J/mol×K	676.32	Joback Method
cpg	423.26	J/mol×K	715.55	Joback Method
cpg	435.38	J/mol×K	754.78	Joback Method
cpg	446.65	J/mol×K	794.00	Joback Method
cpg	457.12	J/mol×K	833.23	Joback Method
dvisc	0.0025386	Pa×s	317.96	Joback Method
dvisc	0.0012089	Pa×s	364.61	Joback Method

dvisc	0.0006812	Pa×s	411.26	Joback Method
dvisc	0.0004315	Pa×s	457.91	Joback Method
dvisc	0.0002974	Pa×s	504.56	Joback Method
dvisc	0.0002183	Pa×s	551.21	Joback Method
dvisc	0.0001681	Pa×s	597.86	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=U374571&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume