

(3-Iodophenyl) methanol, tert.-butyl ether

Inchi:	InChI=1S/C11H15IO/c1-11(2,3)13-8-9-5-4-6-10(12)7-9/h4-7H,8H2,1-3H3
InchiKey:	KGLPPTCGGOENFQ-UHFFFAOYSA-N
Formula:	C11H15IO
SMILES:	CC(C)(C)OCc1cccc(I)c1
Mol. weight [g/mol]:	290.14

Physical Properties

Property code	Value	Unit	Source
gf	100.48	kJ/mol	Joback Method
hf	-109.41	kJ/mol	Joback Method
hfus	16.08	kJ/mol	Joback Method
hvap	53.51	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.606		Crippen Method
mcvol	173.780	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinsol	1577.00		NIST Webbook
tb	595.07	K	Joback Method
tc	840.29	K	Joback Method
tf	335.38	K	Joback Method
vc	0.638	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.47	J/molxK	595.07	Joback Method
cpg	450.46	J/molxK	799.42	Joback Method
cpg	439.26	J/molxK	758.55	Joback Method
cpg	427.14	J/molxK	717.68	Joback Method
cpg	414.01	J/molxK	676.81	Joback Method
cpg	399.82	J/molxK	635.94	Joback Method
cpg	460.80	J/molxK	840.29	Joback Method
dvisc	0.0001607	Paxs	595.07	Joback Method
dvisc	0.0002105	Paxs	551.79	Joback Method

dvisc	0.0002887	Paxs	508.51	Joback Method
dvisc	0.0004197	Paxs	465.22	Joback Method
dvisc	0.0006591	Paxs	421.94	Joback Method
dvisc	0.0011474	Paxs	378.66	Joback Method
dvisc	0.0023046	Paxs	335.38	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=U374578&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

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