

(3-Iodophenyl) methanol, 1-methylpropyl ether

Inchi:	InChI=1S/C11H15IO/c1-3-9(2)13-8-10-5-4-6-11(12)7-10/h4-7,9H,3,8H2,1-2H3
InchiKey:	FOFGDJZWEFFXCG-UHFFFAOYSA-N
Formula:	C11H15IO
SMILES:	CCC(C)OCc1cccc(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	-4.37		Crippen Method
logp	3.606		Crippen Method
mcvol	173.780	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinsol	1606.00		NIST Webbook
tb	597.86	K	Joback Method
tc	833.23	K	Joback Method
tf	317.96	K	Joback Method
vc	0.643	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0006812	Paxs	411.26	Joback Method
dvisc	0.0004315	Paxs	457.91	Joback Method
dvisc	0.0002974	Paxs	504.56	Joback Method
dvisc	0.0002183	Paxs	551.21	Joback Method
dvisc	0.0001681	Paxs	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=U374575&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

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