(3-Iodophenyl) methanol, n-butyl ether

Inchi: InChI=1S/C11H15IO/c1-2-3-7-13-9-10-5-4-6-11(12)8-10/h4-6,8H,2-3,7,9H2,1H3
InchiKey: HRJJHUAJCDKJJS-UHFFFAOYSA-N
Formula: C11H15IO
SMILES: CCCCOCc1cccc(I)c1
Mol. weight [g/mol]: 290.14

Physical Properties

Property code	Value	Unit	Source
gf	97.64	kJ/mol	Joback Method
hf	-100.66	kJ/mol	Joback Method
hfus	23.49	kJ/mol	Joback Method
hvap	54.80	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.608		Crippen Method
mcvol	173.780	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook
tb	598.30	K	Joback Method
tc	828.60	K	Joback Method
tf	332.96	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.01	J/mol×K	598.30	Joback Method
cpg	395.52	J/mol×K	636.68	Joback Method
cpg	409.12	J/mol×K	675.07	Joback Method
cpg	421.86	J/mol×K	713.45	Joback Method
cpg	433.75	J/mol×K	751.83	Joback Method
cpg	444.85	J/mol×K	790.21	Joback Method
cpg	455.18	J/mol×K	828.60	Joback Method
dvisc	0.0019953	Pa×s	332.96	Joback Method

dvisc	0.0010564	Pa×s	377.18	Joback Method
dvisc	0.0006392	Pa×s	421.41	Joback Method
dvisc	0.0004255	Pa×s	465.63	Joback Method
dvisc	0.0003039	Pa×s	509.85	Joback Method
dvisc	0.0002291	Pa×s	554.08	Joback Method
dvisc	0.0001800	Pa×s	598.30	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=U374574&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