(3-Iodophenyl) methanol, n-pentyl ether

Inchi: InChI=1S/C12H17IO/c1-2-3-4-8-14-10-11-6-5-7-12(13)9-11/h5-7,9H,2-4,8,10H2,1H3
InchiKey: WHGFCKHBJHBBKC-UHFFFAOYSA-N
Formula: C12H17IO
SMILES: CCCCCOCc1cccc(I)c1
Mol. weight [g/mol]: 304.17

Physical Properties

Property code	Value	Unit	Source
gf	106.06	kJ/mol	Joback Method
hf	-121.30	kJ/mol	Joback Method
hfus	26.08	kJ/mol	Joback Method
hvap	57.03	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.998		Crippen Method
mcvol	187.870	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
rinpol	1760.00		NIST Webbook
tb	621.18	K	Joback Method
tc	847.05	K	Joback Method
tf	344.23	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.74	J/mol×K	621.18	Joback Method
cpg	496.76	J/mol×K	809.41	Joback Method
cpg	485.09	J/mol×K	771.76	Joback Method
cpg	472.58	J/mol×K	734.12	Joback Method
cpg	459.22	J/mol×K	696.47	Joback Method
cpg	444.95	J/mol×K	658.83	Joback Method
cpg	507.65	J/mol×K	847.05	Joback Method
dvisc	0.0001611	Pa×s	621.18	Joback Method
dvisc	0.0002059	Pa×s	575.02	Joback Method

dvisc	0.0002747	Pa×s	528.86	Joback Method
dvisc	0.0003873	Pa×s	482.70	Joback Method
dvisc	0.0005873	Pa×s	436.55	Joback Method
dvisc	0.0009825	Pa×s	390.39	Joback Method
dvisc	0.0018870	Pa×s	344.23	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=U374579&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