(3-Iodophenyl) methanol, 3-methylbutyl ether

Inchi: InChI=1S/C12H17IO/c1-10(2)6-7-14-9-11-4-3-5-12(13)8-11/h3-5,8,10H,6-7,9H2,1-2H3
InchiKey: UUCSIXSLIAMCNH-UHFFFAOYSA-N
Formula: C12H17IO
SMILES: CC(C)CCOCc1cccc(I)c1
Mol. weight [g/mol]: 304.17

Physical Properties

Property code	Value	Unit	Source
gf	103.62	kJ/mol	Joback Method
hf	-126.58	kJ/mol	Joback Method
hfus	22.56	kJ/mol	Joback Method
hvap	56.64	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.854		Crippen Method
mcvol	187.870	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	1717.00		NIST Webbook
rinpol	1717.00		NIST Webbook
tb	620.74	K	Joback Method
tc	851.41	K	Joback Method
tf	329.23	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.19	J/mol×K	620.74	Joback Method
cpg	445.77	J/mol×K	659.19	Joback Method
cpg	460.36	J/mol×K	697.63	Joback Method
cpg	474.00	J/mol×K	736.08	Joback Method
cpg	486.72	J/mol×K	774.52	Joback Method
cpg	498.57	J/mol×K	812.97	Joback Method
cpg	509.59	J/mol×K	851.41	Joback Method
dvisc	0.0023806	Pa×s	329.23	Joback Method

dvisc	0.0011168	Pa×s	377.81	Joback Method
dvisc	0.0006225	Pa×s	426.40	Joback Method
dvisc	0.0003911	Pa×s	474.99	Joback Method
dvisc	0.0002678	Pa×s	523.57	Joback Method
dvisc	0.0001956	Pa×s	572.15	Joback Method
dvisc	0.0001500	Pa×s	620.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374577&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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