(3-Iodophenyl) methanol, neopentyl ether

Inchi: InChI=1S/C12H17IO/c1-12(2,3)9-14-8-10-5-4-6-11(13)7-10/h4-7H,8-9H2,1-3H3
InchiKey: FYNBFPMURGCMCT-UHFFFAOYSA-N
Formula: C12H17IO
SMILES: CC(C)(C)COCc1cccc(I)c1
Mol. weight [g/mol]: 304.17

Physical Properties

Property code	Value	Unit	Source
gf	108.90	kJ/mol	Joback Method
hf	-130.05	kJ/mol	Joback Method
hfus	18.67	kJ/mol	Joback Method
hvap	55.73	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.854		Crippen Method
mcvol	187.870	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rinpol	1626.00		NIST Webbook
rinpol	1626.00		NIST Webbook
tb	617.95	K	Joback Method
tc	857.94	K	Joback Method
tf	346.65	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.04	J/mol×K	617.95	Joback Method
cpg	449.03	J/mol×K	657.95	Joback Method
cpg	463.87	J/mol×K	697.95	Joback Method
cpg	477.62	J/mol×K	737.95	Joback Method
cpg	490.36	J/mol×K	777.94	Joback Method
cpg	502.16	J/mol×K	817.94	Joback Method
cpg	513.09	J/mol×K	857.94	Joback Method
dvisc	0.0021305	Pa×s	346.65	Joback Method

dvisc	0.0010448	Pa×s	391.87	Joback Method
dvisc	0.0005938	Pa×s	437.08	Joback Method
dvisc	0.0003752	Pa×s	482.30	Joback Method
dvisc	0.0002564	Pa×s	527.52	Joback Method
dvisc	0.0001862	Pa×s	572.73	Joback Method
dvisc	0.0001416	Pa×s	617.95	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=U374580&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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