

(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:	FYNBFBPMURGCMCT-UHFFFAOYSA-N
Formula:	C12H17IO
SMILES:	CC(C)(C)COc1cccc(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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0010448	Paxs	391.87	Joback Method
dvisc	0.0005938	Paxs	437.08	Joback Method
dvisc	0.0003752	Paxs	482.30	Joback Method
dvisc	0.0002564	Paxs	527.52	Joback Method
dvisc	0.0001862	Paxs	572.73	Joback Method
dvisc	0.0001416	Paxs	617.95	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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