

(3-Iodophenyl) methanol, 2-methylbutyl ether

Inchi:	InChI=1S/C12H17IO/c1-3-10(2)8-14-9-11-5-4-6-12(13)7-11/h4-7,10H,3,8-9H2,1-2H3
InchiKey:	ISXGSDJHEUJBAN-UHFFFAOYSA-N
Formula:	C12H17IO
SMILES:	CCC(C)COCc1cccc(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
rinqol	1713.00		NIST Webbook
tb	620.74	K	Joback Method
tc	851.41	K	Joback Method
tf	329.23	K	Joback Method
vc	0.700	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.19	J/molxK	620.74	Joback Method
cpg	445.77	J/molxK	659.19	Joback Method
cpg	460.36	J/molxK	697.63	Joback Method
cpg	474.00	J/molxK	736.08	Joback Method
cpg	486.72	J/molxK	774.52	Joback Method
cpg	498.57	J/molxK	812.97	Joback Method
cpg	509.59	J/molxK	851.41	Joback Method
dvisc	0.0023806	Paxs	329.23	Joback Method
dvisc	0.0011168	Paxs	377.81	Joback Method

dvisc	0.0006225	Paxs	426.40	Joback Method
dvisc	0.0003911	Paxs	474.99	Joback Method
dvisc	0.0002678	Paxs	523.57	Joback Method
dvisc	0.0001956	Paxs	572.15	Joback Method
dvisc	0.0001500	Paxs	620.74	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=U374576&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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