

(3-Iodophenyl) methanol, n-propyl ether

Inchi:	InChI=1S/C10H13IO/c1-2-6-12-8-9-4-3-5-10(11)7-9/h3-5,7H,2,6,8H2,1H3
InchiKey:	XDCWMGLXKFLQ-N-UHFFFAOYSA-N
Formula:	C10H13IO
SMILES:	CCCOc1cccc(I)c1
Mol. weight [g/mol]:	276.11

Physical Properties

Property code	Value	Unit	Source
gf	89.22	kJ/mol	Joback Method
hf	-80.02	kJ/mol	Joback Method
hfus	20.90	kJ/mol	Joback Method
hvap	52.58	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.218		Crippen Method
mvol	159.690	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
rinpol	1553.00		NIST Webbook
tb	575.42	K	Joback Method
tc	810.37	K	Joback Method
tf	321.69	K	Joback Method
vc	0.594	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.91	J/molxK	575.42	Joback Method
cpg	347.59	J/molxK	614.58	Joback Method
cpg	360.40	J/molxK	653.74	Joback Method
cpg	372.39	J/molxK	692.89	Joback Method
cpg	383.57	J/molxK	732.05	Joback Method
cpg	393.99	J/molxK	771.21	Joback Method
cpg	403.68	J/molxK	810.37	Joback Method
dvisc	0.0020909	Paxs	321.69	Joback Method
dvisc	0.0011268	Paxs	363.98	Joback Method

dvisc	0.0006906	Paxs	406.27	Joback Method
dvisc	0.0004642	Paxs	448.56	Joback Method
dvisc	0.0003342	Paxs	490.84	Joback Method
dvisc	0.0002534	Paxs	533.13	Joback Method
dvisc	0.0002001	Paxs	575.42	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=U374573&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
mccvol:	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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