

# 2,3,5-Triiodobenzyl alcohol, n-propyl ether

<b>Inchi:</b>	InChI=1S/C10H11I3O/c1-2-3-14-6-7-4-8(11)5-9(12)10(7)13/h4-5H,2-3,6H2,1H3
<b>InchiKey:</b>	XEXAGXCGKBVGER-UHFFFAOYSA-N
<b>Formula:</b>	C10H11I3O
<b>SMILES:</b>	CCCOc1cc(I)cc(I)c1I
<b>Mol. weight [g/mol]:</b>	527.91

## Physical Properties

Property code	Value	Unit	Source
gf	186.20	kJ/mol	Joback Method
hf	50.78	kJ/mol	Joback Method
hfus	28.94	kJ/mol	Joback Method
hvap	72.64	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	4.427		Crippen Method
mcvol	211.330	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
rinpol	2403.00		NIST Webbook
rinpol	2403.00		NIST Webbook
tb	771.66	K	Joback Method
tc	1062.50	K	Joback Method
tf	462.85	K	Joback Method
vc	0.769	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.13	J/molxK	771.66	Joback Method
cpg	455.74	J/molxK	1014.03	Joback Method
cpg	448.17	J/molxK	965.56	Joback Method
cpg	440.01	J/molxK	917.08	Joback Method
cpg	431.17	J/molxK	868.61	Joback Method
cpg	421.57	J/molxK	820.13	Joback Method
cpg	462.80	J/molxK	1062.50	Joback Method
dvisc	0.0001166	Paxs	771.66	Joback Method

dvisc	0.0001446	Paxs	720.19	Joback Method
dvisc	0.0001853	Paxs	668.72	Joback Method
dvisc	0.0002474	Paxs	617.25	Joback Method
dvisc	0.0003483	Paxs	565.79	Joback Method
dvisc	0.0005250	Paxs	514.32	Joback Method
dvisc	0.0008669	Paxs	462.85	Joback Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U375237&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375237&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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