

# 2,3-Xylenol, 6-ethyl-

<b>Inchi:</b>	InChI=1S/C10H14O/c1-4-9-6-5-7(2)8(3)10(9)11/h5-6,11H,4H2,1-3H3
<b>InchiKey:</b>	DGWHZFYFYSJFCOMZ-UHFFFAOYSA-N
<b>Formula:</b>	C10H14O
<b>SMILES:</b>	CCc1ccc(C)c(C)c1O
<b>Mol. weight [g/mol]:</b>	150.22
<b>CAS:</b>	18441-55-9

## Physical Properties

Property code	Value	Unit	Source
gf	-28.15	kJ/mol	Joback Method
hf	-213.45	kJ/mol	Joback Method
hfus	20.70	kJ/mol	Joback Method
hvap	54.47	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.571		Crippen Method
mvol	133.870	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
tb	513.15 ± 5.00	K	NIST Webbook
tc	766.07	K	Joback Method
tf	326.65 ± 2.00	K	NIST Webbook
tf	325.65 ± 2.00	K	NIST Webbook
tf	326.65 ± 2.00	K	NIST Webbook
vc	0.454	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.96	J/mol×K	545.46	Joback Method
cpg	324.10	J/mol×K	582.23	Joback Method
cpg	336.45	J/mol×K	619.00	Joback Method
cpg	348.06	J/mol×K	655.76	Joback Method
cpg	359.01	J/mol×K	692.53	Joback Method
cpg	369.35	J/mol×K	729.30	Joback Method
cpg	379.14	J/mol×K	766.07	Joback Method

dvisc	0.0014909	Paxs	365.64	Joback Method
dvisc	0.0006933	Paxs	395.61	Joback Method
dvisc	0.0003591	Paxs	425.58	Joback Method
dvisc	0.0002028	Paxs	455.55	Joback Method
dvisc	0.0001229	Paxs	485.52	Joback Method
dvisc	0.0000790	Paxs	515.49	Joback Method
dvisc	0.0000533	Paxs	545.46	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=C18441559&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18441559&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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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