

# 2,3,6-Trimethylbenzoic acid

Inchi:	InChI=1S/C10H12O2/c1-6-4-5-7(2)9(8(6)3)10(11)12/h4-5H,1-3H3,(H,11,12)
InchiKey:	JRUKSSBDIZXQDX-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	Cc1ccc(C)c(C([O])=O)c1C
Mol. weight [g/mol]:	164.20
CAS:	2529-36-4

## Physical Properties

Property code	Value	Unit	Source
chs	-5174.52 ± 0.84	kJ/mol	NIST Webbook
hf	-371.20 ± 1.90	kJ/mol	NIST Webbook
hfs	-475.60 ± 1.90	kJ/mol	NIST Webbook
hsub	104.40 ± 0.20	kJ/mol	NIST Webbook
hsub	104.40	kJ/mol	NIST Webbook
hsub	104.40 ± 0.20	kJ/mol	NIST Webbook
log10ws	-7.53		Crippen Method
logp	2.183		Crippen Method
mcvol	133.290	ml/mol	McGowan Method
rinpol	1402.00		NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	103.60 ± 0.20	kJ/mol	325.00	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{\text{vp}}) = A + B/(T + C)$
Coeff. A	1.38828e+01

Coeff. B	-4.38457e+03
Coeff. C	-8.84900e+01
Temperature range (K), min.	411.00
Temperature range (K), max.	600.03

## 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=C2529364&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2529364&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<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>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices

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