# (E)-1-(2,3,6-trimethylphenyl)buta-1,3-diene (TPB, 1)

**Other names:** tert-1-(2,3,6-Trimethylphenyl)buta-1,3-diene
**Inchi:** InChI=1S/C13H16/c1-5-6-7-13-11(3)9-8-10(2)12(13)4/h5-9H,1H2,2-4H3/b7-6+
**InchiKey:** CBIAGJZZVUQDOC-VOTSOKGWSA-N
**Formula:** C13H16
**SMILES:** C=CC=Cc1c(C)ccc(C)c1C
**Mol. weight [g/mol]:** 172.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 310.16 | kJ/mol | Joback Method |
| hf | 133.12 | kJ/mol | Joback Method |
| hfus | 21.22 | kJ/mol | Joback Method |
| hvap | 48.08 | kJ/mol | Joback Method |
| log10ws | -4.41 | | Crippen Method |
| logp | 3.811 | | Crippen Method |
| mcvol | 161.670 | ml/mol | McGowan Method |
| pc | 2298.11 | kPa | Joback Method |
| ripol | 1832.00 | | NIST Webbook |
| ripol | 1832.00 | | NIST Webbook |
| ripol | 1832.00 | | NIST Webbook |
| tb | 539.30 | K | Joback Method |
| tc | 752.61 | K | Joback Method |
| tf | 293.41 | K | Joback Method |
| vc | 0.617 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 356.77 | J/mol×K | 539.30 | Joback Method |
| cpg | 372.37 | J/mol×K | 574.85 | Joback Method |
| cpg | 387.09 | J/mol×K | 610.40 | Joback Method |
| cpg | 400.98 | J/mol×K | 645.96 | Joback Method |
| cpg | 414.08 | J/mol×K | 681.51 | Joback Method |
| cpg | 426.43 | J/mol×K | 717.06 | Joback Method |

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|---|---|---|---|---|
| cpg | 438.09 | J/mol×K | 752.61 | Joback Method |
| dvisc | 0.0012135 | Pa×s | 293.41 | Joback Method |
| dvisc | 0.0006976 | Pa×s | 334.39 | Joback Method |
| dvisc | 0.0004526 | Pa×s | 375.37 | Joback Method |
| dvisc | 0.0003197 | Pa×s | 416.36 | Joback Method |
| dvisc | 0.0002404 | Pa×s | 457.34 | Joback Method |
| dvisc | 0.0001894 | Pa×s | 498.32 | Joback Method |
| dvisc | 0.0001548 | Pa×s | 539.30 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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=U357257&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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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