

tert-Butyl acrylate

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| Other names: | 1,1-dimethylethyl 2-propenoate 2-Propenoic acid, 1,1-dimethylethyl ester Acrylic acid, tert-butyl ester t-Butyl acrylate tert-butyl 2-propenoate |
| Inchi: | InChI=1S/C7H12O2/c1-5-6(8)9-7(2,3)4/h5H,1H2,2-4H3 |
| InchiKey: | ISXSCDLOGDJUNJ-UHFFFAOYSA-N |
| Formula: | C7H12O2 |
| SMILES: | C=CC(=O)OC(C)(C)C |
| Mol. weight [g/mol]: | 128.17 |
| CAS: | 1663-39-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -135.18 | kJ/mol | Joback Method |
| hf | -315.93 | kJ/mol | Joback Method |
| hfus | 7.98 | kJ/mol | Joback Method |
| hvap | 38.37 | kJ/mol | Joback Method |
| log10ws | -1.58 | | Crippen Method |
| logp | 1.514 | | Crippen Method |
| mcvol | 112.630 | ml/mol | McGowan Method |
| pc | 3145.56 | kPa | Joback Method |
| tb | 429.30 | K | Joback Method |
| tc | 621.15 | K | Joback Method |
| tf | 241.47 | K | Joback Method |
| vc | 0.421 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 287.01 | J/molxK | 621.15 | Joback Method |
| cpg | 236.97 | J/molxK | 461.28 | Joback Method |
| cpg | 248.07 | J/molxK | 493.25 | Joback Method |
| cpg | 258.61 | J/molxK | 525.23 | Joback Method |

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|-------|-----------|---------|--------|--|
| cpg | 268.60 | J/molxK | 557.20 | Joback Method |
| cpg | 278.06 | J/molxK | 589.18 | Joback Method |
| cpg | 225.27 | J/molxK | 429.30 | Joback Method |
| dvisc | 0.0043009 | Paxs | 241.47 | Joback Method |
| dvisc | 0.0020951 | Paxs | 272.78 | Joback Method |
| dvisc | 0.0011835 | Paxs | 304.08 | Joback Method |
| dvisc | 0.0007438 | Paxs | 335.38 | Joback Method |
| dvisc | 0.0005060 | Paxs | 366.69 | Joback Method |
| dvisc | 0.0003658 | Paxs | 398.00 | Joback Method |
| dvisc | 0.0002772 | Paxs | 429.30 | Joback Method |
| rho1 | 884.13 | kg/m3 | 293.15 | Densities and volumetric properties of (acetonitrile + alkyl acrylate monomer) binary mixtures at temperatures from 293.15 K to 318.15 K |
| rho1 | 879.66 | kg/m3 | 298.15 | Densities and volumetric properties of (acetonitrile + alkyl acrylate monomer) binary mixtures at temperatures from 293.15 K to 318.15 K |
| rho1 | 875.20 | kg/m3 | 303.15 | Densities and volumetric properties of (acetonitrile + alkyl acrylate monomer) binary mixtures at temperatures from 293.15 K to 318.15 K |
| rho1 | 870.74 | kg/m3 | 308.15 | Densities and volumetric properties of (acetonitrile + alkyl acrylate monomer) binary mixtures at temperatures from 293.15 K to 318.15 K |
| rho1 | 866.28 | kg/m3 | 313.15 | Densities and volumetric properties of (acetonitrile + alkyl acrylate monomer) binary mixtures at temperatures from 293.15 K to 318.15 K |

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|-----|--------|-------------------|--------|--|
| rho | 861.82 | kg/m ³ | 318.15 | Densities and volumetric properties of (acetonitrile + alkyl acrylate monomer) binary mixtures at temperatures from 293.15 K to 318.15 K |
| rho | 884.13 | kg/m ³ | 293.15 | Temperature and concentration dependence of volumetric properties of (tetrahydrofuran + methyl acrylate, or + ethyl acrylate, or + n-butyl acrylate, or + tert-butyl acrylate) binary mixtures |
| rho | 879.66 | kg/m ³ | 298.15 | Temperature and concentration dependence of volumetric properties of (tetrahydrofuran + methyl acrylate, or + ethyl acrylate, or + n-butyl acrylate, or + tert-butyl acrylate) binary mixtures |
| rho | 875.20 | kg/m ³ | 303.15 | Temperature and concentration dependence of volumetric properties of (tetrahydrofuran + methyl acrylate, or + ethyl acrylate, or + n-butyl acrylate, or + tert-butyl acrylate) binary mixtures |
| rho | 870.74 | kg/m ³ | 308.15 | Temperature and concentration dependence of volumetric properties of (tetrahydrofuran + methyl acrylate, or + ethyl acrylate, or + n-butyl acrylate, or + tert-butyl acrylate) binary mixtures |

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|------|--------|-------|--------|--|
| rho1 | 866.28 | kg/m3 | 313.15 | Temperature and concentration dependence of volumetric properties of (tetrahydrofuran + methyl acrylate, or + ethyl acrylate, or + n-butyl acrylate, or + tert-butyl acrylate) binary mixtures |
| rho1 | 861.82 | kg/m3 | 318.15 | Temperature and concentration dependence of volumetric properties of (tetrahydrofuran + methyl acrylate, or + ethyl acrylate, or + n-butyl acrylate, or + tert-butyl acrylate) binary mixtures |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.89075e+01 |
| Coeff. B | -5.07474e+03 |
| Coeff. C | -6.56080e+01 |
| Temperature range (K), min. | 338.15 |
| Temperature range (K), max. | 438.86 |

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Densities and volumetric properties of (acetonitrile + alkyl acrylate monomer) binary mixtures as a function of temperature and concentration

<https://www.doi.org/10.1016/j.jct.2016.08.026>

Temperature and concentration dependence of volumetric properties of (tetrahydrofuran + methyl acrylate, or + ethyl acrylate, or + n-butyl acrylate, or + tert-butyl acrylate) binary mixtures:

<https://www.doi.org/10.1016/j.jct.2016.10.042>

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=C1663394&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 |
| pvap: | Vapor pressure |
| rho: | Liquid Density |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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