# Isobutyl radical

**Inchi:** InChI=1S/C4H9/c1-4(2)3/h4H,1H2,2-3H3
**InchiKey:** KTOQRRDVVIDEAA-UHFFFAOYSA-N
**Formula:** C4H9
**SMILES:** [CH2]C(C)C
**Mol. weight [g/mol]:** 57.11
**CAS:** 4630-45-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ea | 0.05 ± 0.12 | eV | NIST Webbook |
| gf | 32.74 | kJ/mol | Joback Method |
| hf | 70.00 ± 2.00 | kJ/mol | NIST Webbook |
| hfus | 4.27 | kJ/mol | Joback Method |
| hvap | 23.96 | kJ/mol | Joback Method |
| ie | 7.93 ± 0.03 | eV | NIST Webbook |
| ie | 8.31 ± 0.03 | eV | NIST Webbook |
| ie | 8.01 ± 0.05 | eV | NIST Webbook |
| log10ws | -0.87 | | Crippen Method |
| logp | 1.476 | | Crippen Method |
| mcvol | 65.070 | ml/mol | McGowan Method |
| pc | 4162.33 | kPa | Joback Method |
| tb | 289.78 | K | Joback Method |
| tc | 451.90 | K | Joback Method |
| tf | 136.21 | K | Joback Method |
| vc | 0.244 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 89.53 | J/mol×K | 289.78 | Joback Method |
| cpg | 124.64 | J/mol×K | 424.88 | Joback Method |
| cpg | 118.33 | J/mol×K | 397.86 | Joback Method |
| cpg | 111.68 | J/mol×K | 370.84 | Joback Method |
| cpg | 104.68 | J/mol×K | 343.82 | Joback Method |

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|---|---|---|---|---|
| cpg | 97.30 | J/mol×K | 316.80 | Joback Method |
| cpg | 130.63 | J/mol×K | 451.90 | Joback Method |
| dvisc | 0.0001712 | Pa×s | 289.78 | Joback Method |
| dvisc | 0.0001875 | Pa×s | 264.19 | Joback Method |
| dvisc | 0.0002092 | Pa×s | 238.59 | Joback Method |
| dvisc | 0.0002398 | Pa×s | 213.00 | Joback Method |
| dvisc | 0.0002853 | Pa×s | 187.40 | Joback Method |
| dvisc | 0.0003585 | Pa×s | 161.81 | Joback Method |
| dvisc | 0.0004910 | Pa×s | 136.21 | Joback Method |

# Sources

**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=C4630459&Units=SI

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**ea:** Electron affinity
**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
**ie:** Ionization energy
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume

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