# Propanenitrile, 3-(1-methylethoxy)-

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|---|---|
| **Other names:** | Propionitrile, 3-isopropoxy- |
| | «beta»-Isopropoxypropionitrile |
| | 3-Isopropoxypropionitrile |
| | Beta-iso-propoxypropionitrile |
| | 3-isopropoxypropiononitrile |
| **Inchi:** | InChI=1S/C6H11NO/c1-6(2)8-5-3-4-7/h6H,3,5H2,1-2H3 |
| **InchiKey:** | BMSYXLRQGIFLFO-UHFFFAOYSA-N |
| **Formula:** | C6H11NO |
| **SMILES:** | CC(C)OCCC#N |
| **Mol. weight [g/mol]:** | 113.16 |
| **CAS:** | 110-47-4 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 25.38 | kJ/mol | Joback Method |
| hf | -139.79 | kJ/mol | Joback Method |
| hfus | 10.47 | kJ/mol | Joback Method |
| hvap | 41.45 | kJ/mol | Joback Method |
| log10ws | -1.40 | | Crippen Method |
| logp | 1.325 | | Crippen Method |
| mcvol | 102.650 | ml/mol | McGowan Method |
| pc | 2992.59 | kPa | Joback Method |
| rinpol | 879.00 | | NIST Webbook |
| rinpol | 879.00 | | NIST Webbook |
| tb | 460.74 | K | Joback Method |
| tc | 653.11 | K | Joback Method |
| tf | 229.60 | K | Joback Method |
| vc | 0.409 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 211.29 | J/mol×K | 460.74 | Joback Method |
| cpg | 220.73 | J/mol×K | 492.80 | Joback Method |

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|---|---|---|---|---|
| cpg | 229.82 | J/mol×K | 524.86 | Joback Method |
| cpg | 238.57 | J/mol×K | 556.93 | Joback Method |
| cpg | 246.98 | J/mol×K | 588.99 | Joback Method |
| cpg | 255.04 | J/mol×K | 621.05 | Joback Method |
| cpg | 262.77 | J/mol×K | 653.11 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C110474&Units=SI |
| **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 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |