

2-Propanamine, N-(1-methylethylidene)-

Inchi: InChI=1S/C6H13N/c1-5(2)7-6(3)4/h5H,1-4H3
InchiKey: UCJOAMOXKLJGST-UHFFFAOYSA-N
Formula: C6H13N
SMILES: CC(C)=NC(C)C
Mol. weight [g/mol]: 99.17
CAS: 3332-08-9

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------------|--------|----------------|
| hf | -100.02 | kJ/mol | Joback Method |
| hvap | 31.96 | kJ/mol | Joback Method |
| ie | 8.40 ± 0.20 | eV | NIST Webbook |
| log10ws | -1.61 | | Crippen Method |
| logp | 1.876 | | Crippen Method |
| mvol | 101.080 | ml/mol | McGowan Method |
| pc | 2811.36 | kPa | Joback Method |
| tb | 412.80 | K | Joback Method |
| tc | 608.80 | K | Joback Method |

Sources

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=C3332089&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

hf: Enthalpy of formation 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 |

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