

Linalyl 2-methylbutanoate

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| Other names: | linalyl 2-methylbutyrate |
| Inchi: | InChI=1S/C15H26O2/c1-7-13(5)14(16)17-15(6,8-2)11-9-10-12(3)4/h8,10,13H,2,7,9,11H2 |
| InchiKey: | MLJNGBGMEMFTPV-UHFFFAOYSA-N |
| Formula: | C15H26O2 |
| SMILES: | <chem>C=CC(C)(CCC=C(C)C)OC(=O)C(C)CC</chem> |
| Mol. weight [g/mol]: | 238.37 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 1.41 | kJ/mol | Joback Method |
| hf | -378.90 | kJ/mol | Joback Method |
| hfus | 24.07 | kJ/mol | Joback Method |
| hvap | 55.82 | kJ/mol | Joback Method |
| log10ws | -4.54 | | Crippen Method |
| logp | 4.267 | | Crippen Method |
| mcvol | 221.050 | ml/mol | McGowan Method |
| pc | 1618.07 | kPa | Joback Method |
| rinpol | 1450.00 | | NIST Webbook |
| rinpol | 1461.00 | | NIST Webbook |
| ripol | 1695.00 | | NIST Webbook |
| ripol | 1695.00 | | NIST Webbook |
| tb | 615.94 | K | Joback Method |
| tc | 805.63 | K | Joback Method |
| tf | 297.59 | K | Joback Method |
| vc | 0.845 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 581.43 | J/molxK | 615.94 | Joback Method |
| cpg | 599.22 | J/molxK | 647.55 | Joback Method |
| cpg | 616.05 | J/molxK | 679.17 | Joback Method |
| cpg | 631.97 | J/molxK | 710.78 | Joback Method |
| cpg | 647.03 | J/molxK | 742.40 | Joback Method |

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|-----|--------|---------|--------|---------------|
| cpg | 661.27 | J/mol×K | 774.01 | Joback Method |
| cpg | 674.74 | J/mol×K | 805.63 | 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=R288187&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-----------------|---|
| 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 |
| rinpola: | Non-polar retention indices |
| ripola: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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