

2(3H)-Furanone, dihydro-5-pentyl-

| | |
|-----------------------------|---|
| Other names: | (.+/-)-«gamma»-Nonalactone (3H)-Dihydro-5-pentyl-2-furanone 1,4-Nonalolide 4-Hydroxynonanoic acid lactone 4-Hydroxynonanoic acid, «gamma»-lactone 4-Nonanolide 4-Pentylbutanolide 5-Pentyl-«gamma»-lactone 5-Pentyl-dihydrofuran-2(3H)-one 5-pentyl-dihydro-2(3H)-furanone 5-pentyl-dihydrofuran-2(3H)-one («gamma»-nonalactone) Aldehyde C-18 Cocos aldehyde Dihydro-5-pentyl-2(3H)-furanon Nonan-1,4-olide Nonanoic acid, 4-hydroxy-, «gamma»-lactone Prunolide dihydro-5-pentyl-2(3H)-furanone nonan-4-olide «gamma»-Amyl-«gamma»-butyrolactone «gamma»-Amylbutyrolactone «gamma»-Nonalacton «gamma»-Nonalactone «gamma»-Nonanoic lactone «gamma»-Nonanolactone «gamma»-Nonanolide «gamma»-n-Amylbutyrolactone |
| Inchi: | InChI=1S/C9H16O2/c1-2-3-4-5-8-6-7-9(10)11-8/h8H,2-7H2,1H3 |
| InchiKey: | OALYTRUKMRCXNH-UHFFFAOYSA-N |
| Formula: | C9H16O2 |
| SMILES: | CCCCC1CCC(=O)O1 |
| Mol. weight [g/mol]: | 156.22 |
| CAS: | 104-61-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------|------|--------|
|---------------|-------|------|--------|

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|---------------------|--------------|--------|----------------|
| gf | -147.26 | kJ/mol | Joback Method |
| hf | -438.31 | kJ/mol | Joback Method |
| hfus | 20.49 | kJ/mol | Joback Method |
| h _{vap} | 70.30 ± 0.20 | kJ/mol | NIST Webbook |
| log10w _s | -2.46 | | Crippen Method |
| logp | 2.272 | | Crippen Method |
| m _{cvol} | 134.250 | ml/mol | McGowan Method |
| pc | 2841.41 | kPa | Joback Method |
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| tb | 515.37 | K | Joback Method |
| tc | 722.96 | K | Joback Method |
| tf | 296.88 | K | Joback Method |
| vc | 0.508 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 339.38 | J/mol×K | 549.97 | Joback Method |
| cpg | 410.16 | J/mol×K | 722.96 | Joback Method |
| cpg | 397.48 | J/mol×K | 688.36 | Joback Method |
| cpg | 384.07 | J/mol×K | 653.76 | Joback Method |
| cpg | 369.92 | J/mol×K | 619.16 | Joback Method |
| cpg | 355.02 | J/mol×K | 584.57 | Joback Method |
| cpg | 322.99 | J/mol×K | 515.37 | Joback Method |

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|-------|-------|--------|--------|--|
| hvapt | 70.50 | kJ/mol | 298.15 | Vapor pressures and enthalpies of vaporization of a series of .gamma. and .delta.-lactones by correlation gas chromatography |
| pvap | 0.07 | kPa | 353.20 | Vapour pressures and enthalpies of vapourization of a series of the c-lactones |
| pvap | 0.04 | kPa | 342.80 | Vapour pressures and enthalpies of vapourization of a series of the c-lactones |
| pvap | 0.05 | kPa | 348.40 | Vapour pressures and enthalpies of vapourization of a series of the c-lactones |
| pvap | 0.03 | kPa | 338.00 | Vapour pressures and enthalpies of vapourization of a series of the c-lactones |
| pvap | 0.10 | kPa | 358.10 | Vapour pressures and enthalpies of vapourization of a series of the c-lactones |
| pvap | 0.14 | kPa | 363.40 | Vapour pressures and enthalpies of vapourization of a series of the c-lactones |
| pvap | 0.02 | kPa | 333.10 | Vapour pressures and enthalpies of vapourization of a series of the c-lactones |
| pvap | 0.01 | kPa | 328.20 | Vapour pressures and enthalpies of vapourization of a series of the c-lactones |

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|------|----------|-----|--------|--|
| pvap | 8.80e-03 | kPa | 323.20 | Vapour pressures and enthalpies of vapourization of a series of the c-lactones |
| pvap | 5.74e-03 | kPa | 318.10 | Vapour pressures and enthalpies of vapourization of a series of the c-lactones |
| pvap | 3.91e-03 | kPa | 313.10 | Vapour pressures and enthalpies of vapourization of a series of the c-lactones |
| pvap | 2.11e-03 | kPa | 306.00 | Vapour pressures and enthalpies of vapourization of a series of the c-lactones |
| pvap | 1.23e-03 | kPa | 300.00 | Vapour pressures and enthalpies of vapourization of a series of the c-lactones |
| pvap | 8.50e-04 | kPa | 296.20 | Vapour pressures and enthalpies of vapourization of a series of the c-lactones |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 394.70 | K | 0.80 | NIST Webbook |

Sources

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<http://webbook.nist.gov/cgi/cbook.cgi?ID=C104610&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

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