

Benzene, 1,1',1'',1'''-(1-propyn-1-yl-3-ylidyne)tetrakis-

Other names:

Propyne, tetraphenyl-

Inchi: InChI=1S/C27H20/c1-5-13-23(14-6-1)21-22-27(24-15-7-2-8-16-24,25-17-9-3-10-18-25)2

InchiKey: VXFRQOLYYOGJNU-UHFFFAOYSA-N

Formula: C27H20

SMILES: C(#CC(c1cccc1)(c1cccc1)c1cccc1)c1cccc1

Mol. weight [g/mol]: 344.45

CAS: 20143-13-9

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------------|---------|----------------|
| gf | 831.74 | kJ/mol | Joback Method |
| hf | 609.06 | kJ/mol | Joback Method |
| hfus | 37.56 | kJ/mol | Joback Method |
| hvap | 85.66 | kJ/mol | Joback Method |
| ie | 8.20 ± 0.08 | eV | NIST Webbook |
| log10ws | -7.31 | | Crippen Method |
| logp | 6.073 | | Crippen Method |
| mcvol | 287.650 | ml/mol | McGowan Method |
| pc | 1878.90 | kPa | Joback Method |
| tb | 929.65 | K | Joback Method |
| tc | 1232.95 | K | Joback Method |
| tf | 608.25 | K | Joback Method |
| vc | 1.067 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 854.62 | J/molxK | 929.65 | Joback Method |
| cpg | 872.10 | J/molxK | 980.20 | Joback Method |
| cpg | 888.11 | J/molxK | 1030.75 | Joback Method |
| cpg | 903.01 | J/molxK | 1081.30 | Joback Method |
| cpg | 917.15 | J/molxK | 1131.85 | Joback Method |
| cpg | 930.90 | J/molxK | 1182.40 | Joback Method |
| cpg | 944.61 | J/molxK | 1232.95 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C20143139&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |
| ie: | Ionization energy |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mconvol: | 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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