

Benzene, 1-fluoro-4-(2-phenylethyl)-

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| Other names: | Bibenzyl, 4-fluoro-4-Fluorobibenzyl 1-(4-Fluorophenyl)-2-phenylethane L-(4-Fluorophenyl)-2-phenylethane |
| Inchi: | InChI=1S/C14H13F/c15-14-10-8-13(9-11-14)7-6-12-4-2-1-3-5-12/h1-5,8-11H,6-7H2 |
| InchiKey: | LGAWAQNSZFCGMP-UHFFFAOYSA-N |
| Formula: | C14H13F |
| SMILES: | Fc1ccc(CCc2ccccc2)cc1 |
| Mol. weight [g/mol]: | 200.25 |
| CAS: | 370-76-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------------|---------|----------------|
| gf | 87.38 | kJ/mol | Joback Method |
| hf | -66.81 | kJ/mol | Joback Method |
| hfus | 22.79 | kJ/mol | Joback Method |
| hvap | 51.16 | kJ/mol | Joback Method |
| ie | 8.80 ± 0.10 | eV | NIST Webbook |
| log10ws | -4.22 | | Crippen Method |
| logp | 3.611 | | Crippen Method |
| mcvol | 162.370 | ml/mol | McGowan Method |
| pc | 2603.08 | kPa | Joback Method |
| tb | 577.33 | K | Joback Method |
| tc | 805.90 | K | Joback Method |
| tf | 313.49 | K | Joback Method |
| vc | 0.622 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 380.31 | J/molxK | 577.33 | Joback Method |
| cpg | 396.84 | J/molxK | 615.42 | Joback Method |
| cpg | 412.20 | J/molxK | 653.52 | Joback Method |
| cpg | 426.45 | J/molxK | 691.61 | Joback Method |

| | | | | |
|-----|--------|---------|--------|---------------|
| cpg | 439.65 | J/mol×K | 729.71 | Joback Method |
| cpg | 451.86 | J/mol×K | 767.80 | Joback Method |
| cpg | 463.15 | J/mol×K | 805.90 | 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=C370763&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |
| hvp: | 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 |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/70-285-8/Benzene-1-fluoro-4-2-phenylethyl.pdf>

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