

Lactarazulene

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|-----------------------------|----------------------------------------------------------------------------|
| Inchi: | InChI=1S/C15H16/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h5-9H,1H2,2-4H3 |
| InchiKey: | KFLXZUPIDNPCSD-UHFFFAOYSA-N |
| Formula: | C15H16 |
| SMILES: | <chem>C=C(C)c1ccc(C)c2ccc(C)c-2c1</chem> |
| Mol. weight [g/mol]: | 196.29 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 344.88 | kJ/mol | Joback Method |
| hf | 155.90 | kJ/mol | Joback Method |
| hfus | 21.91 | kJ/mol | Joback Method |
| hvap | 54.30 | kJ/mol | Joback Method |
| log10ws | -5.68 | | Crippen Method |
| logp | 4.441 | | Crippen Method |
| mcvol | 174.690 | ml/mol | McGowan Method |
| pc | 2311.39 | kPa | Joback Method |
| rinpol | 1796.00 | | NIST Webbook |
| rinpol | 1792.00 | | NIST Webbook |
| rinpol | 1796.00 | | NIST Webbook |
| ripol | 2430.00 | | NIST Webbook |
| tb | 599.76 | K | Joback Method |
| tc | 828.44 | K | Joback Method |
| tf | 339.77 | K | Joback Method |
| vc | 0.671 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 417.47 | J/molxK | 599.76 | Joback Method |
| cpg | 433.79 | J/molxK | 637.87 | Joback Method |
| cpg | 449.04 | J/molxK | 675.99 | Joback Method |
| cpg | 463.30 | J/molxK | 714.10 | Joback Method |
| cpg | 476.64 | J/molxK | 752.21 | Joback Method |
| cpg | 489.14 | J/molxK | 790.33 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=R614209&Units=SI |

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 |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| ripol: | Polar retention indices |
| 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/75-202-4/Lactarazulene.pdf>

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