

As-Indacene, dodecahydro-4-(1-octylnonyl)-

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|-----------------------------|---|
| Other names: | 5-(1'-n-Octylnonyl)-(dodecahydro(as)indacene) 9-(4-as-Perhydroindacenyl)heptadecane 9-(4'-as-Decahydroindacenyl)heptadecane |
| Inchi: | InChI=1S/C29H54/c1-3-5-7-9-11-13-17-24(18-14-12-10-8-6-4-2)29-23-25-19-15-20-26(2) |
| InchiKey: | JSKCOAYGYKRYTA-UHFFFAOYSA-N |
| Formula: | C29H54 |
| SMILES: | CCCCCCCCC(CCCCCCCC)C1CC2CCCC2C2CCCC12 |
| Mol. weight [g/mol]: | 402.74 |
| CAS: | 55530-51-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 321.39 | kJ/mol | Joback Method |
| hf | -487.93 | kJ/mol | Joback Method |
| hfus | 57.59 | kJ/mol | Joback Method |
| hvap | 79.40 | kJ/mol | Joback Method |
| log10ws | -10.20 | | Crippen Method |
| logp | 9.956 | | Crippen Method |
| mcvol | 386.890 | ml/mol | McGowan Method |
| pc | 773.75 | kPa | Joback Method |
| tb | 886.17 | K | Joback Method |
| tc | 1087.30 | K | Joback Method |
| tf | 436.37 | K | Joback Method |
| vc | 1.498 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1391.85 | J/molxK | 886.17 | Joback Method |
| cpg | 1417.64 | J/molxK | 919.69 | Joback Method |
| cpg | 1442.01 | J/molxK | 953.21 | Joback Method |
| cpg | 1465.08 | J/molxK | 986.74 | Joback Method |
| cpg | 1486.96 | J/molxK | 1020.26 | Joback Method |
| cpg | 1507.75 | J/molxK | 1053.78 | Joback Method |

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|-------|-----------|---------|---------|---------------|
| cpg | 1527.57 | J/mol×K | 1087.30 | Joback Method |
| dvisc | 0.0032450 | Paxs | 436.37 | Joback Method |
| dvisc | 0.0018478 | Paxs | 511.34 | Joback Method |
| dvisc | 0.0012151 | Paxs | 586.30 | Joback Method |
| dvisc | 0.0008788 | Paxs | 661.27 | Joback Method |
| dvisc | 0.0006789 | Paxs | 736.24 | Joback Method |
| dvisc | 0.0005501 | Paxs | 811.20 | Joback Method |
| dvisc | 0.0004618 | Paxs | 886.17 | 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=C55530513&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| 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 |
| 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/79-988-9/As-Indacene-dodecahydro-4-1-octylonyl.pdf>

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