

9H-Pyrido[3,4-b]indole

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|-----------------------------|---|
| Other names: | 2,9-Diazafluorene 9H-.beta.-carboline 9H-Beta-carboline Carbazoline Norharman Norharmane «beta»-Carboline Â«betaÂ»-Carboline |
| Inchi: | InChI=1S/C11H8N2/c1-2-4-10-8(3-1)9-5-6-12-7-11(9)13-10/h1-7,13H |
| InchiKey: | AIFRHYZBTHREPW-UHFFFAOYSA-N |
| Formula: | C11H8N2 |
| SMILES: | <chem>c1ccc2c(c1)[nH]c1cnccc12</chem> |
| Mol. weight [g/mol]: | 168.19 |
| CAS: | 244-63-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------------|--------|--------------------------------------|
| ie | 7.99 ± 0.06 | eV | NIST Webbook |
| log10ws | -3.73 | | Aqueous Solubility Prediction Method |
| logp | 2.234 | | Crippen Method |
| mvol | 127.430 | ml/mol | McGowan Method |
| rinpol | 2009.00 | | NIST Webbook |
| rinpol | 2005.00 | | NIST Webbook |
| rinpol | 2005.00 | | NIST Webbook |
| rinpol | 2009.00 | | NIST Webbook |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-------|--------|-----------------|--------------|
| hfust | 25.50 | kJ/mol | 471.50 | NIST Webbook |
| hfust | 25.50 | kJ/mol | 471.50 | NIST Webbook |

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|------|----------|-----|--------|--|
| psub | 5.03e-05 | kPa | 374.10 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |
| psub | 1.74e-05 | kPa | 363.80 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |
| psub | 2.56e-05 | kPa | 367.90 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |
| psub | 2.72e-05 | kPa | 368.10 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |
| psub | 3.37e-05 | kPa | 370.30 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |

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|------|----------|-----|--------|--|
| psub | 4.16e-05 | kPa | 371.40 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |
| psub | 4.16e-05 | kPa | 371.50 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |
| psub | 5.70e-06 | kPa | 352.80 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |
| psub | 5.45e-05 | kPa | 374.40 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |
| psub | 7.53e-05 | kPa | 378.20 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |

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|------|----------|-----|--------|--|
| psub | 1.03e-04 | kPa | 381.80 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |
| psub | 1.07e-04 | kPa | 382.00 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |
| psub | 1.08e-04 | kPa | 382.20 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |
| psub | 1.41e-04 | kPa | 385.40 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |
| psub | 1.55e-04 | kPa | 385.90 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |

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|------|----------|-----|--------|--|
| psub | 2.18e-04 | kPa | 389.20 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |
| psub | 2.29e-04 | kPa | 389.40 | Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique |

Sources

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|--|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C244633&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Vapor pressures and sublimation enthalpies of seven heteroatomic aromatic hydrocarbons measured using the Knudsen effusion technique: McGowan Method: | https://www.doi.org/10.1016/j.jct.2010.01.014 |
| Aromatic Solubility Prediction Method: | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

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|-----------------|---|
| hfust: | Enthalpy of fusion at a given temperature |
| ie: | Ionization energy |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| psub: | Sublimation pressure |
| rinpola: | Non-polar retention indices |

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