

# Diazeno, bis(4-ethoxyphenyl)-, 1-oxide

|                      |                                                                                                                                                                                                                                                                                                                                            |
|----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Azoxybenzene, 4,4'-diethoxy-<br>p,p'-Azoxyphenetole<br>4,4'-Azoxydiphenetole<br>4,4'-Azoxyphenetole<br>4,4'-Bis(ethoxy)azoxybenzene<br>4,4'-Diethoxyazoxybenzene<br>p-Azoxyphenetole<br>p,p'-Azoxydiphenetole<br>p,p'-Diethoxyazoxybenzene<br>Azoxyphenetole<br>NSC 142006<br>p,p'-Diethoxyazoxybenzene<br>PAP<br>Phenetole, 4,4'-azoxydi- |
| Inchi:               | InChI=1S/C16H18N2O3/c1-3-20-15-9-5-13(6-10-15)17-18(19)14-7-11-16(12-8-14)21-4-2                                                                                                                                                                                                                                                           |
| InchiKey:            | QUICZVHSJNKDBL-UHFFFAOYSA-N                                                                                                                                                                                                                                                                                                                |
| Formula:             | C16H18N2O3                                                                                                                                                                                                                                                                                                                                 |
| SMILES:              | CCOc1ccc(N=[N+](O-))c2ccc(OCC)cc2cc1                                                                                                                                                                                                                                                                                                       |
| Mol. weight [g/mol]: | 286.33                                                                                                                                                                                                                                                                                                                                     |
| CAS:                 | 4792-83-0                                                                                                                                                                                                                                                                                                                                  |

## Physical Properties

| Property code | Value           | Unit   | Source         |
|---------------|-----------------|--------|----------------|
| chs           | -8705.00 ± 1.50 | kJ/mol | NIST Webbook   |
| chs           | -8822.80        | kJ/mol | NIST Webbook   |
| chs           | -8822.80        | kJ/mol | NIST Webbook   |
| hf            | -37.40 ± 3.70   | kJ/mol | NIST Webbook   |
| hfs           | -163.60 ± 2.60  | kJ/mol | NIST Webbook   |
| hfs           | -45.60          | kJ/mol | NIST Webbook   |
| hfs           | -45.86          | kJ/mol | NIST Webbook   |
| hsub          | 126.20 ± 2.70   | kJ/mol | NIST Webbook   |
| hsub          | 126.20 ± 2.70   | kJ/mol | NIST Webbook   |
| ie            | 7.20            | eV     | NIST Webbook   |
| ie            | 7.65            | eV     | NIST Webbook   |
| log10ws       | -4.48           |        | Crippen Method |
| logp          | 4.410           |        | Crippen Method |
| mcvol         | 222.050         | ml/mol | McGowan Method |

# Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source       |
|---------------|--------|---------|-----------------|--------------|
| cpl           | 607.00 | J/mol×K | 430.00          | NIST Webbook |
| hfust         | 27.00  | kJ/mol  | 406.50          | NIST Webbook |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                   |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4792830&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4792830&amp;Units=SI</a> |

## Legend

|                 |                                                          |
|-----------------|----------------------------------------------------------|
| <b>chs:</b>     | Standard solid enthalpy of combustion                    |
| <b>cpl:</b>     | Liquid phase heat capacity                               |
| <b>hf:</b>      | Enthalpy of formation at standard conditions             |
| <b>hfs:</b>     | Solid phase enthalpy of formation at standard conditions |
| <b>hfust:</b>   | Enthalpy of fusion at a given temperature                |
| <b>hsub:</b>    | Enthalpy of sublimation at standard conditions           |
| <b>ie:</b>      | Ionization energy                                        |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l                       |
| <b>logp:</b>    | Octanol/Water partition coefficient                      |
| <b>mcvol:</b>   | McGowan's characteristic volume                          |

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