

Carbonic acid, but-2-yn-1-yl tetradecyl ester

Inchi: InChI=1S/C19H34O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-18-22-19(20)21-17-6-4-2/h3,5,
InchiKey: YDESNQMXTHNGAK-UHFFFAOYSA-N
Formula: C19H34O3
SMILES: CC#CCOC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 310.47

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -27.02 | kJ/mol | Joback Method |
| hf | -540.21 | kJ/mol | Joback Method |
| hfus | 52.06 | kJ/mol | Joback Method |
| hvap | 71.61 | kJ/mol | Joback Method |
| log10ws | -6.50 | | Crippen Method |
| logp | 5.864 | | Crippen Method |
| mcvol | 283.280 | ml/mol | McGowan Method |
| pc | 1228.56 | kPa | Joback Method |
| rinpola | 2227.00 | | NIST Webbook |
| rinpola | 2227.00 | | NIST Webbook |
| tb | 741.83 | K | Joback Method |
| tc | 922.92 | K | Joback Method |
| tf | 504.38 | K | Joback Method |
| vc | 1.103 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 835.90 | J/mol×K | 741.83 | Joback Method |
| cpg | 854.28 | J/mol×K | 772.01 | Joback Method |
| cpg | 871.75 | J/mol×K | 802.19 | Joback Method |
| cpg | 888.32 | J/mol×K | 832.37 | Joback Method |
| cpg | 903.99 | J/mol×K | 862.56 | Joback Method |
| cpg | 918.79 | J/mol×K | 892.74 | Joback Method |
| cpg | 932.72 | J/mol×K | 922.92 | 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=U383209&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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