

2-Aminopent-4-enoic acid, N-(but-2-yn-1-yloxycarbonyl)-, octyl ester

Inchi: InChI=1S/C18H29NO4/c1-4-7-9-10-11-12-15-22-17(20)16(13-6-3)19-18(21)23-14-8-5-2/
InchiKey: SNCLXLDSZSQDGP-UHFFFAOYSA-N
Formula: C18H29NO4
SMILES: C=CCC(N=C(O)OCC#CC)C(=O)OCCCCCCCC
Mol. weight [g/mol]: 323.43

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -479.22 | kJ/mol | Joback Method |
| hvap | 88.39 | kJ/mol | Joback Method |
| log10ws | -4.55 | | Crippen Method |
| logp | 3.789 | | Crippen Method |
| mcvol | 276.440 | ml/mol | McGowan Method |
| pc | 1356.63 | kPa | Joback Method |
| rinpol | 2262.00 | | NIST Webbook |
| rinpol | 2262.00 | | NIST Webbook |
| tb | 883.93 | K | Joback Method |
| tc | 1086.45 | K | 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=U393195&Units=SI>

Legend

hf: Enthalpy of formation 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 |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

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