

Thiocyanic acid, (2-benzothiazolylthio)methyl ester

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| Other names: | (benzothiazol-2-ylthio)methyl thiocyanate 2-(Thiocyanomethylthio)benzothiazole 2-[(Thiocyanatomethyl)thio]benzothiazole Alentisan Benthiazole Busan Busan 1030 Busan 15 Busan 30 Busan 30-1 Busan 30A Busan 30I Busan 70 Busan 71 Busan 72 Busan 72A Delsan 30 Ichiban KVK 733059 Sancelant TMB Superdavloxan TCMTB |
| Inchi: | InChI=1S/C9H6N2S3/c10-5-12-6-13-9-11-7-3-1-2-4-8(7)14-9/h1-4H,6H2 |
| InchiKey: | TUBQDCKAWGHZPF-UHFFFAOYSA-N |
| Formula: | C9H6N2S3 |
| SMILES: | N#CSCSc1nc2cccc2s1 |
| Mol. weight [g/mol]: | 238.35 |
| CAS: | 21564-17-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.70 | | Crippen Method |
| logp | 3.560 | | Crippen Method |
| mcvol | 159.160 | ml/mol | McGowan Method |
| rinpol | 2162.00 | | NIST Webbook |
| rinpol | 2162.00 | | NIST Webbook |

Sources

| | |
|--|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C21564170&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| Solubility of Organic Biocides in Supercritical CO₂ and CO₂ + Cosolvent Mixtures: | https://www.doi.org/10.1021/je0255473 |

Legend

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|----------------------------|--|
| log₁₀ws: | Log ₁₀ of Water solubility in mol/l |
| log_p: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| rinpol: | Non-polar retention indices |

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