

# N-(2-methyl-2-methylsulfanylpropylidene)hydroxy

|                      |                                                |
|----------------------|------------------------------------------------|
| Inchi:               | InChI=1S/C5H11NOS/c1-5(2,8-3)4-6-7/h4,7H,1-3H3 |
| InchiKey:            | ZFGMCJAXIZTVJA-UHFFFAOYSA-N                    |
| Formula:             | C5H11NOS                                       |
| SMILES:              | CSC(C)(C)C=NO                                  |
| Mol. weight [g/mol]: | 133.22                                         |
| CAS:                 | 1646-75-9                                      |

## Physical Properties

| Property code | Value     | Unit   | Source                                                     |
|---------------|-----------|--------|------------------------------------------------------------|
| log10ws       | -7.41e-03 |        | Cheméo Relay (1.0)                                         |
| logp          | 1.588     |        | Crippen Method                                             |
| mcvol         | 109.210   | ml/mol | McGowan Method                                             |
| tf            | 294.15    | K      | Jean-Claude Bradley Open Melting Point Dataset (2014, CC0) |

## Sources

|                                                             |                                                                                                                                                                                         |
|-------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method:                                             | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                                                                       |
| Cheméo Relay (1.0):                                         |                                                                                                                                                                                         |
| Cheméo Relay (1.0, beta):                                   |                                                                                                                                                                                         |
| Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): | <a href="https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637">https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637</a> |
| Joback Method:                                              | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                   |
| McGowan Method:                                             | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                                                                   |
| Crippen Method:                                             | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                                                               |

## Legend

|          |                                     |
|----------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l  |
| logp:    | Octanol/Water partition coefficient |
| mcvol:   | McGowan's characteristic volume     |
| tf:      | Normal melting (fusion) point       |

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