# Phenol, 3,5-dimethyl-4-(methylsulfonyl)-, methylcarbamate

**Other names:** Phenol, 3,5-dimethyl-4-(methylsulfonyl)-, methylcarbamate
Carbamic acid, methyl-, 4-(methylsulfonyl)-3,5-xylyl ester
Ba 51-084786
Bay 37344 sulfone
Bayer 37344 Sulfone
BAY 41790
Carbamic acid, methyl-, 3,5-dimethyl-4-(methylsulfonyl)phenyl ester
ENT 25825
3,5-Xylenol, 4-(methylsulfonyl)-, methylcarbamate
Methiocarb sulfone

**Inchi:** InChI=1S/C11H15NO4S/c1-7-5-9(16-11(13)12-3)6-8(2)10(7)17(4,14)15/h5-6H,1-4H3,(H,

**InchiKey:** RJBJMKAMQIOAML-UHFFFAOYSA-N

**Formula:** C11H15NO4S

**SMILES:** CNC(=O)Oc1cc(C)c(S(C)(=O)=O)c(C)c1

**Mol. weight [g/mol]:** 257.31

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 36.38 | kJ/mol | Joback Method |
| log10ws | -3.26 | | Cheméo Relay (1.0) |
| logp | 1.425 | | Crippen Method |
| mcvol | 187.600 | ml/mol | McGowan Method |
| tf | 419.05 | K | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 478.63 | J/mol×K | 666.94 | Joback Method |
| cpg | 492.03 | J/mol×K | 701.09 | Joback Method |
| cpg | 504.61 | J/mol×K | 735.25 | Joback Method |
| cpg | 516.35 | J/mol×K | 769.40 | Joback Method |
| cpg | 527.24 | J/mol×K | 803.56 | Joback Method |
| cpg | 537.27 | J/mol×K | 837.71 | Joback Method |
| cpg | 546.43 | J/mol×K | 871.86 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2179251&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **tf:** | Normal melting (fusion) point |