

Methyl 2-isothiocyanato-4-(methylthio)butyrate

Inchi: InChI=1S/C7H11NO2S2/c1-10-7(9)6(8-5-11)3-4-12-2/h6H,3-4H2,1-2H3
InchiKey: HNBACGFGPNFPAF-UHFFFAOYSA-N
Formula: C7H11NO2S2
SMILES: COC(=O)C(CCSC)N=C=S
Mol. weight [g/mol]: 205.30
CAS: 21055-47-0

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -111.95 | kJ/mol | Joback Method |
| hvap | 57.20 | kJ/mol | Joback Method |
| log10ws | -1.54 | | Crippen Method |
| logp | 1.384 | | Crippen Method |
| mcvol | 151.010 | ml/mol | McGowan Method |
| pc | 3096.73 | kPa | Joback Method |
| tb | 650.14 | K | Joback Method |
| tc | 889.72 | K | Joback Method |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C21055470&Units=SI>
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

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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

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