Isothiocyanatoacetaldehyde dimethyl acetal

Inchi: InChI=1S/C5H9NO2S/c1-7-5(8-2)3-6-4-9/h5H,3H2,1-2H3
InchiKey: LMLTWPRCKDMKLQ-UHFFFAOYSA-N
Formula: C5H9NO2S
SMILES: COC(CN=C=S)OC
Mol. weight [g/mol]: 147.19
CAS: 75052-04-9

Physical Properties

Property code	Value	Unit	Source
hf	-132.18	kJ/mol	Joback Method
hvap	41.60	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.708		Crippen Method
mcvol	110.780	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
tb	504.15	K	Joback Method
tc	722.79	K	Joback Method

Sources

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=C75052049&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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