

2-(Dichloromethyl)dimethylsilyloxybut-3-yne

Inchi: InChI=1S/C7H12Cl2OSi/c1-5-6(2)10-11(3,4)7(8)9/h1,6-7H,2-4H3
InchiKey: KCXLVLPMPDPWQW-UHFFFAOYSA-N
Formula: C7H12Cl2OSi
SMILES: C#CC(C)O[Si](C)(C)C(Cl)Cl
Mol. weight [g/mol]: 211.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.80		Crippen Method
logp	2.573		Crippen Method
rinpol	711.00		NIST Webbook
rinpol	711.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299449&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/21-157-4/2-Dichloromethyl-dimethylsilyloxybut-3-yne.pdf>

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