

methyl N-[methyl-[methyl-(1-methylsulfanylethylideneam

Inchi:	InChI=1S/C10H18N4O4S3/c1-7(19-5)11-17-9(15)13(3)21-14(4)10(16)18-12-8(2)20-6/h1
InchiKey:	XDOTVMNBCQVZKG-UHFFFAOYSA-N
Formula:	C10H18N4O4S3
SMILES:	CSC(C)=NOC(=O)N(C)SN(C)C(=O)ON=C(C)SC
Mol. weight [g/mol]:	354.48
CAS:	59669-26-0

Physical Properties

Property code	Value	Unit	Source
logp	3.079		Crippen Method
mcvol	247.010	ml/mol	McGowan Method
tf	446.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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