

sulfometuron-methyl

Inchi:	InChI=1S/C15H16N4O5S/c1-9-8-10(2)17-14(16-9)18-15(21)19-25(22,23)12-7-5-4-6-11(1
InchiKey:	ZDXMLEQEMNLCQG-UHFFFAOYSA-N
Formula:	C15H16N4O5S
SMILES:	<chem>COC(=O)c1ccccc1S(=O)(=O)NC(=O)Nc1nc(C)cc(C)n1</chem>
Mol. weight [g/mol]:	364.38
CAS:	74222-97-2

Physical Properties

Property code	Value	Unit	Source
hf	-650.18	kJ/mol	Cheméo Relay (1.0)
ie	8.40	eV	Cheméo Relay (1.0)
log10ws	-3.50		Cheméo Relay (1.0)
logp	1.390		Crippen Method
mcvol	251.710	ml/mol	McGowan Method
pc	2607.08	kPa	Cheméo Relay (1.0, beta)
tb	675.11	K	Cheméo Relay (1.0)
tf	475.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Jean-Claude Bradley Open Melting
Point Dataset (2014, CC0):
McGowan Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

<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):

Legend

hf: Enthalpy of formation at standard conditions

ie:	Ionization energy
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
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.cheméo.com/cid/106-574-7/sulfometuron-methyl.pdf>

Generated by Cheméo on 2026-10-31 16:53:42.214121565 +0000 UTC m=+89335.140958845.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.