

METHANESULFONIC ANHYDRIDE

Other names:	Methanesulfonic acid, anhydride Mesyl anhydride Methanesulphonic anhydride
Inchi:	InChI=1S/C2H6O5S2/c1-8(3,4)7-9(2,5)6/h1-2H3
InchiKey:	IZDROVVXIHRYMH-UHFFFAOYSA-N
Formula:	C2H6O5S2
SMILES:	CS(=O)(=O)OS(C)(=O)=O
Mol. weight [g/mol]:	174.20

Physical Properties

Property code	Value	Unit	Source
hf	-866.07	kJ/mol	Cheméo Relay (1.0)
hfus	24.88	kJ/mol	Joback Method
ie	11.00	eV	Cheméo Relay (1.0)
logp	-1.078		Crippen Method
mcvol	101.090	ml/mol	McGowan Method
tb	508.25	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.54	J/mol×K	363.14	Joback Method
cpg	184.20	J/mol×K	390.37	Joback Method
cpg	190.79	J/mol×K	417.60	Joback Method
cpg	197.31	J/mol×K	444.82	Joback Method
cpg	203.73	J/mol×K	472.05	Joback Method
cpg	210.02	J/mol×K	499.28	Joback Method
cpg	216.17	J/mol×K	526.51	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7143013&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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