

Benzenesulfonic acid, methyl ester

Other names:	Methyl benzenesulfonate 20ND3-5 Methyl ester of benzenesulphonic acid methyl benzenesulphonate
Inchi:	InChI=1S/C7H8O3S/c1-10-11(8,9)7-5-3-2-4-6-7/h2-6H,1H3
InchiKey:	CZXGXYBOQYQXQD-UHFFFAOYSA-N
Formula:	C7H8O3S
SMILES:	COS(=O)(=O)c1ccccc1
Mol. weight [g/mol]:	172.20
CAS:	80-18-2

Physical Properties

Property code	Value	Unit	Source
gf	-453.07	kJ/mol	Joback Method
hf	-536.85	kJ/mol	Joback Method
hfus	20.49	kJ/mol	Joback Method
hvap	54.50	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	1.022		Crippen Method
mcvol	119.690	ml/mol	McGowan Method
pc	4952.36	kPa	Joback Method
tb	456.44	K	Joback Method
tc	661.30	K	Joback Method
tf	255.86	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.08	J/mol×K	456.44	Joback Method
cpg	242.90	J/mol×K	490.58	Joback Method
cpg	254.16	J/mol×K	524.73	Joback Method
cpg	264.85	J/mol×K	558.87	Joback Method
cpg	274.97	J/mol×K	593.02	Joback Method

cpg	284.50	J/mol×K	627.16	Joback Method
cpg	293.46	J/mol×K	661.30	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	423.00	K	2.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C80182&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/30-338-3/Benzenesulfonic-acid-methyl-ester.pdf>

Generated by Cheméo on 2025-12-23 16:22:58.321860803 +0000 UTC m=+6255175.851901470.

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