

Benzonitrile, 4-(methylsulfonyl)-

Other names:	Benzonitrile, p-(methylsulfonyl)- 4-(Methylsulfonyl)benzonitrile p-Methanesulfonylbenzonitrile 4-(CH ₃ SO ₂)-C ₆ H ₄ -CN
Inchi:	InChI=1S/C8H7NO2S/c1-12(10,11)8-4-2-7(6-9)3-5-8/h2-5H,1H3
InchiKey:	FARXIDYHJAANGP-UHFFFAOYSA-N
Formula:	C ₈ H ₇ NO ₂ S
SMILES:	CS(=O)(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]:	181.21
CAS:	22821-76-7

Physical Properties

Property code	Value	Unit	Source
affp	798.70	kJ/mol	NIST Webbook
basg	768.00	kJ/mol	NIST Webbook
gf	-216.10	kJ/mol	Joback Method
hf	-271.86	kJ/mol	Joback Method
hfus	23.01	kJ/mol	Joback Method
hvap	65.45	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	0.962		Crippen Method
mcvol	129.290	ml/mol	McGowan Method
pc	4216.56	kPa	Joback Method
tb	563.96	K	Joback Method
tc	787.24	K	Joback Method
tf	322.41	K	Joback Method
vc	0.527	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.12	J/mol×K	563.96	Joback Method
cpg	285.69	J/mol×K	601.17	Joback Method
cpg	295.57	J/mol×K	638.39	Joback Method

cpg	304.76	J/mol×K	675.60	Joback Method
cpg	313.25	J/mol×K	712.81	Joback Method
cpg	321.07	J/mol×K	750.02	Joback Method
cpg	328.20	J/mol×K	787.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22821767&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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