N-Methylbenzenesulfonamide

Other names: Benzenesulfonamide, N-methyl-
N-methylbenzenesulphonamide
Inchi: InChI=1S/C7H9NO2S/c1-8-11(9,10)7-5-3-2-4-6-7/h2-6,8H,1H3
InchiKey: SVDVKEBISAOWJT-UHFFFAOYSA-N
Formula: C7H9NO2S
SMILES: CNS(=O)(=O)c1ccccc1
Mol. weight [g/mol]: 171.22
CAS: 5183-78-8

Physical Properties

Property code	Value	Unit	Source
gf	-258.68	kJ/mol	Joback Method
hf	-351.16	kJ/mol	Joback Method
hfus	24.40	kJ/mol	Joback Method
hvap	58.52	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	0.595		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	5168.28	kPa	Joback Method
tb	484.19	K	Joback Method
tc	692.60	K	Joback Method
tf	286.29	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.52	J/mol×K	484.19	Joback Method
cpg	264.06	J/mol×K	518.93	Joback Method
cpg	275.88	J/mol×K	553.66	Joback Method
cpg	286.99	J/mol×K	588.40	Joback Method
cpg	297.39	J/mol×K	623.13	Joback Method
cpg	307.10	J/mol×K	657.87	Joback Method
cpg	316.12	J/mol×K	692.60	Joback Method

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=C5183788&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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