

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

Physical Properties

Property code	Value	Unit	Source
hf	-202.51	kJ/mol	Cheméo Relay (1.0)
hfus	24.40	kJ/mol	Joback Method
ie	9.43	eV	Cheméo Relay (1.0)
log10ws	-1.19		Cheméo Relay (1.0)
logp	0.595		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
tb	573.89	K	Cheméo Relay (1.0)
tf	364.59	K	Cheméo Relay (1.0)

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/ci990307I
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=C5183788&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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