

O-NITROBENZENESULFONAMIDE

Other names:	2-Nitrobenzenesulphonamide
Inchi:	InChI=1S/C6H6N2O4S/c7-13(11,12)6-4-2-1-3-5(6)8(9)10/h1-4H,(H2,7,11,12)
InchiKey:	GNDKYAWHEKZHPJ-UHFFFAOYSA-N
Formula:	C6H6N2O4S
SMILES:	NS(=O)(=O)c1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	202.19

Physical Properties

Property code	Value	Unit	Source
hf	-211.94	kJ/mol	Cheméo Relay (1.0)
hfus	32.88	kJ/mol	Joback Method
hvap	88.92	kJ/mol	Cheméo Relay (1.0)
ie	10.02	eV	Cheméo Relay (1.0)
log10ws	-2.76		Cheméo Relay (1.0)
logp	0.242		Crippen Method
mcvol	127.130	ml/mol	McGowan Method
tb	580.80	K	Cheméo Relay (1.0)
tf	411.75	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.69	J/mol×K	640.49	Joback Method
cpg	311.72	J/mol×K	682.19	Joback Method
cpg	320.82	J/mol×K	723.89	Joback Method
cpg	329.01	J/mol×K	765.59	Joback Method
cpg	336.31	J/mol×K	807.30	Joback Method
cpg	342.72	J/mol×K	849.00	Joback Method
cpg	348.26	J/mol×K	890.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C5455594&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization 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

Latest version available from:

<https://www.chemeo.com/cid/123-604-4/O-NITROBENZENESULFONAMIDE.pdf>

Generated by Cheméo on 2026-07-21 10:34:15.099923584 +0000 UTC m=+141150.941808954.

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