

Benzenesulfonamide, N-(4-nitrophenyl)-

Other names:	N-p-Nitro-phenyl-benzene-sulfonamide
Inchi:	InChI=1S/C12H10N2O4S/c15-14(16)11-8-6-10(7-9-11)13-19(17,18)12-4-2-1-3-5-12/h1-9
InchiKey:	SWSJPCDGYPPCS-UHFFFAOYSA-N
Formula:	C12H10N2O4S
SMILES:	O=[N+]([O-])c1ccc(NS(=O)(=O)c2ccccc2)cc1
Mol. weight [g/mol]:	278.28
CAS:	1829-81-8

Physical Properties

Property code	Value	Unit	Source
gf	-78.25	kJ/mol	Joback Method
hf	-240.06	kJ/mol	Joback Method
hfus	42.37	kJ/mol	Joback Method
hvap	89.18	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.396		Crippen Method
mcvol	187.910	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
tb	782.09	K	Joback Method
tc	1038.28	K	Joback Method
tf	525.19	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.42	J/mol×K	782.09	Joback Method
cpg	516.18	J/mol×K	824.79	Joback Method
cpg	526.57	J/mol×K	867.49	Joback Method
cpg	535.64	J/mol×K	910.19	Joback Method
cpg	543.45	J/mol×K	952.89	Joback Method
cpg	550.06	J/mol×K	995.59	Joback Method
cpg	555.53	J/mol×K	1038.28	Joback Method

Sources

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=C1829818&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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