

H2N-NO2

Inchi: InChI=1S/H2N2O2/c1-2(3)4/h1H2
InchiKey: SFDJOSRHYKHMOK-UHFFFAOYSA-N
Formula: H2N2O2
SMILES: N[N+](=O)[O-]
Mol. weight [g/mol]: 62.03
CAS: 7782-94-7

Physical Properties

Property code	Value	Unit	Source
affp	757.40	kJ/mol	NIST Webbook
basg	725.00	kJ/mol	NIST Webbook
gf	51.12	kJ/mol	Joback Method
hf	-20.30	kJ/mol	Joback Method
hfus	12.31	kJ/mol	Joback Method
hvap	42.83	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	-0.863		Crippen Method
mcvol	38.260	ml/mol	McGowan Method
pc	7574.60	kPa	Joback Method
tb	423.77	K	Joback Method
tc	657.01	K	Joback Method
tf	316.63	K	Joback Method
vc	0.146	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	68.71	J/mol×K	423.77	Joback Method
cpg	72.20	J/mol×K	462.64	Joback Method
cpg	75.47	J/mol×K	501.52	Joback Method
cpg	78.54	J/mol×K	540.39	Joback Method
cpg	81.41	J/mol×K	579.26	Joback Method
cpg	84.08	J/mol×K	618.14	Joback Method
cpg	86.57	J/mol×K	657.01	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=C7782947&Units=SI

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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