

1-Propanamine, N-nitro-N-propyl-

Other names:	Dipropylamine, N-nitro- Dipropylnitramine Di-n-propylnitramine
Inchi:	InChI=1S/C6H14N2O2/c1-3-5-7(6-4-2)8(9)10/h3-6H2,1-2H3
InchiKey:	ZUNKPQMZTMJVVOB-UHFFFAOYSA-N
Formula:	C6H14N2O2
SMILES:	CCCN(CCC)[N+](=O)[O-]
Mol. weight [g/mol]:	146.19
CAS:	4164-29-8

Physical Properties

Property code	Value	Unit	Source
chl	-4188.60	kJ/mol	NIST Webbook
gf	145.97	kJ/mol	Joback Method
hf	-110.40	kJ/mol	Joback Method
hfus	25.68	kJ/mol	Joback Method
hvap	47.58	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.300		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
tb	500.96	K	Joback Method
tc	700.04	K	Joback Method
tf	333.46	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.43	J/molxK	500.96	Joback Method
cpg	295.06	J/molxK	534.14	Joback Method
cpg	307.01	J/molxK	567.32	Joback Method
cpg	318.32	J/molxK	600.50	Joback Method
cpg	329.01	J/molxK	633.68	Joback Method

cpg	339.10	J/mol×K	666.86	Joback Method
cpg	348.62	J/mol×K	700.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4164298&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
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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