1-Propanamine, N-nitro-

Other names: n-Propylnitramine
Inchi: InChI=1S/C3H8N2O2/c1-2-3-4-5(6)7/h4H,2-3H2,1H3
InchiKey: MCROFHCOHPROAE-UHFFFAOYSA-N
Formula: C3H8N2O2
SMILES: CCCN[N+](=O)[O-]
Mol. weight [g/mol]: 104.11
CAS: 627-07-6

Physical Properties

Property code	Value	Unit	Source
chl	-2216.00	kJ/mol	NIST Webbook
gf	99.32	kJ/mol	Joback Method
hf	-62.54	kJ/mol	Joback Method
hfus	19.99	kJ/mol	Joback Method
hvap	45.30	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	0.178		Crippen Method
mcvol	80.530	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
tb	470.05	K	Joback Method
tc	682.15	K	Joback Method
tf	319.84	K	Joback Method
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.55	J/mol×K	470.05	Joback Method
cpg	178.17	J/mol×K	505.40	Joback Method
cpg	186.32	J/mol×K	540.75	Joback Method
cpg	194.03	J/mol×K	576.10	Joback Method
cpg	201.32	J/mol×K	611.45	Joback Method
cpg	208.18	J/mol×K	646.80	Joback Method
cpg	214.65	J/mol×K	682.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C627076&Units=SI
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

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