1-Propanamine, N,2-dimethyl-N-nitro-

Inchi: InChI=1S/C5H12N2O2/c1-5(2)4-6(3)7(8)9/h5H,4H2,1-3H3
InchiKey: VHQJQNRZBRJXCE-UHFFFAOYSA-N
Formula: C5H12N2O2
SMILES: CC(C)CN(C)[N+](=O)[O-]
Mol. weight [g/mol]: 132.16
CAS: 53951-45-4

Physical Properties

Property code	Value	Unit	Source
gf	135.11	kJ/mol	Joback Method
hf	-95.04	kJ/mol	Joback Method
hfus	19.57	kJ/mol	Joback Method
hvap	44.97	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	0.766		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
tb	477.64	K	Joback Method
tc	684.04	K	Joback Method
tf	295.65 ± 1.00	K	NIST Webbook
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.15	J/mol×K	477.64	Joback Method
cpg	252.10	J/mol×K	512.04	Joback Method
cpg	263.38	J/mol×K	546.44	Joback Method
cpg	274.03	J/mol×K	580.84	Joback Method
cpg	284.06	J/mol×K	615.24	Joback Method
cpg	293.50	J/mol×K	649.64	Joback Method
cpg	302.38	J/mol×K	684.04	Joback Method

Sources

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=C53951454&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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