Formamide, N-propyl-

Other names: n-C3H7NHCHO
Inchi: InChI=1S/C4H9NO/c1-2-3-5-4-6/h4H,2-3H2,1H3,(H,5,6)
InchiKey: SUUDTPGCUKBECW-UHFFFAOYSA-N
Formula: C4H9NO
SMILES: CCCNC=O
Mol. weight [g/mol]: 87.12
CAS: 6281-94-3

Physical Properties

Property code	Value	Unit	Source
affp	878.40	kJ/mol	NIST Webbook
basg	847.40	kJ/mol	NIST Webbook
gf	-27.33	kJ/mol	Joback Method
hf	-158.00	kJ/mol	Joback Method
hfus	13.50	kJ/mol	Joback Method
hvap	37.65	kJ/mol	Joback Method
log10ws	-0.46		Crippen Method
logp	0.142		Crippen Method
mcvol	78.770	ml/mol	McGowan Method
pc	4356.87	kPa	Joback Method
rinpol	934.00		NIST Webbook
rinpol	934.00		NIST Webbook
tb	389.75	K	Joback Method
tc	569.07	K	Joback Method
tf	229.50	K	Joback Method
vc	0.311	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.69	J/mol×K	389.75	Joback Method
cpg	153.64	J/mol×K	419.64	Joback Method
cpg	161.27	J/mol×K	449.52	Joback Method
cpg	168.59	J/mol×K	479.41	Joback Method

cpg	175.60	J/mol×K	509.30	Joback Method
cpg	182.31	J/mol×K	539.18	Joback Method
cpg	188.74	J/mol×K	569.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6281943&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume