Formamide, N-hexyl

Inchi: InChI=1S/C7H15NO/c1-2-3-4-5-6-8-7-9/h7H,2-6H2,1H3,(H,8,9)
InchiKey: NHTXRWUMLXSOGJ-UHFFFAOYSA-N
Formula: C7H15NO
SMILES: CCCCCCNC=O
Mol. weight [g/mol]: 129.20

Physical Properties

Property code	Value	Unit	Source
gf	-2.07	kJ/mol	Joback Method
hf	-219.92	kJ/mol	Joback Method
hfus	21.27	kJ/mol	Joback Method
hvap	44.33	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.313		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
rinpol	1274.00		NIST Webbook
rinpol	1274.00		NIST Webbook
tb	458.39	K	Joback Method
tc	634.13	K	Joback Method
tf	263.31	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.53	J/mol×K	458.39	Joback Method
cpg	272.15	J/mol×K	487.68	Joback Method
cpg	283.28	J/mol×K	516.97	Joback Method
cpg	293.94	J/mol×K	546.26	Joback Method
cpg	304.14	J/mol×K	575.55	Joback Method
cpg	313.90	J/mol×K	604.84	Joback Method
cpg	323.23	J/mol×K	634.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R50654&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

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