Propanamide, N-hexyl-

Other names: Propionamide, N-hexyl-
N-Hexylpropionamide
Inchi: InChI=1S/C9H19NO/c1-3-5-6-7-8-10-9(11)4-2/h3-8H2,1-2H3,(H,10,11)
InchiKey: WVNFFHLXDXOSGO-UHFFFAOYSA-N
Formula: C9H19NO
SMILES: CCCCCCNC(=O)CC
Mol. weight [g/mol]: 157.25
CAS: 10264-24-1

Physical Properties

Property code	Value	Unit	Source
gf	-14.63	kJ/mol	Joback Method
hf	-288.20	kJ/mol	Joback Method
hfus	25.76	kJ/mol	Joback Method
hvap	48.81	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.093		Crippen Method
mcvol	149.220	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1353.00		NIST Webbook
rinpol	1353.00		NIST Webbook
tb	509.36	K	Joback Method
tc	686.41	K	Joback Method
tf	293.78	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.12	J/mol×K	509.36	Joback Method
cpg	360.93	J/mol×K	538.87	Joback Method
cpg	374.14	J/mol×K	568.38	Joback Method
cpg	386.77	J/mol×K	597.89	Joback Method
cpg	398.85	J/mol×K	627.40	Joback Method

cpg	410.39	J/mol×K	656.91	Joback Method
cpg	421.39	J/mol×K	686.41	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10264241&Units=SI

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