1-Pyrroline, 2-hexanoyl

Inchi: InChI=1S/C10H17NO/c1-2-3-4-7-10(12)9-6-5-8-11-9/h2-8H2,1H3
InchiKey: AOTAURKLJAXOEJ-UHFFFAOYSA-N
Formula: C10H17NO
SMILES: CCCCCC(=O)C1=NCCC1
Mol. weight [g/mol]: 167.25

Physical Properties

Property code	Value	Unit	Source
gf	85.77	kJ/mol	Joback Method
hf	-164.21	kJ/mol	Joback Method
hfus	22.09	kJ/mol	Joback Method
hvap	52.33	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.371		Crippen Method
mcvol	148.150	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	1319.00		NIST Webbook
rinpol	1319.00		NIST Webbook
tb	559.86	K	Joback Method
tc	771.58	K	Joback Method
tf	352.35	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.68	J/mol×K	559.86	Joback Method
cpg	390.46	J/mol×K	595.15	Joback Method
cpg	406.30	J/mol×K	630.43	Joback Method
cpg	421.22	J/mol×K	665.72	Joback Method
cpg	435.24	J/mol×K	701.01	Joback Method
cpg	448.38	J/mol×K	736.29	Joback Method
cpg	460.68	J/mol×K	771.58	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=R66223&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