2-Propionyl-1,4,5,6-tetrahydropyridine

Inchi: InChI=1S/C8H13NO/c1-2-8(10)7-5-3-4-6-9-7/h5,9H,2-4,6H2,1H3
InchiKey: DOGZYNACXGUDFW-UHFFFAOYSA-N
Formula: C8H13NO
SMILES: CCC(=O)C1=CCCCN1
Mol. weight [g/mol]: 139.19
CAS: 80933-74-0

Physical Properties

Property code	Value	Unit	Source
gf	27.76	kJ/mol	Joback Method
hf	-162.25	kJ/mol	Joback Method
hfus	19.26	kJ/mol	Joback Method
hvap	48.60	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.233		Crippen Method
mcvol	119.970	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	1239.00		NIST Webbook
tb	513.22	K	Joback Method
tc	736.23	K	Joback Method
tf	359.78	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.78	J/mol×K	513.22	Joback Method
cpg	278.36	J/mol×K	550.39	Joback Method
cpg	292.14	J/mol×K	587.56	Joback Method
cpg	305.13	J/mol×K	624.73	Joback Method
cpg	317.35	J/mol×K	661.89	Joback Method
cpg	328.82	J/mol×K	699.06	Joback Method
cpg	339.57	J/mol×K	736.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80933740&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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