2-Propionyl-3,4,5,6-tetrahydropyridine

Inchi: InChI=1S/C8H13NO/c1-2-8(10)7-5-3-4-6-9-7/h2-6H2,1H3
InchiKey: GGYSXLMPBBMRHY-UHFFFAOYSA-N
Formula: C8H13NO
SMILES: CCC(=O)C1=NCCCC1
Mol. weight [g/mol]: 139.19
CAS: 80933-75-1

Physical Properties

Property code	Value	Unit	Source
gf	56.83	kJ/mol	Joback Method
hf	-129.09	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	48.05	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	1.590		Crippen Method
mcvol	119.970	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	1148.00		NIST Webbook
rinpol	1148.00		NIST Webbook
tb	518.37	K	Joback Method
tc	745.63	K	Joback Method
tf	326.29	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.17	J/mol×K	518.37	Joback Method
cpg	296.36	J/mol×K	556.25	Joback Method
cpg	311.62	J/mol×K	594.12	Joback Method
cpg	325.96	J/mol×K	632.00	Joback Method
cpg	339.40	J/mol×K	669.87	Joback Method
cpg	351.95	J/mol×K	707.75	Joback Method
cpg	363.61	J/mol×K	745.63	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=C80933751&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