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

Other names: Ethanone, 1-(1,4,5,6-tetrahydro-2-pyridinyl)-
Inchi: InChI=1S/C7H11NO/c1-6(9)7-4-2-3-5-8-7/h4,8H,2-3,5H2,1H3
InchiKey: HRAOWRVFLSYJKN-UHFFFAOYSA-N
Formula: C7H11NO
SMILES: CC(=O)C1=CCCCN1
Mol. weight [g/mol]: 125.17
CAS: 25343-57-1

Physical Properties

Property code	Value	Unit	Source
gf	19.34	kJ/mol	Joback Method
hf	-141.61	kJ/mol	Joback Method
hfus	16.67	kJ/mol	Joback Method
hvap	46.37	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	0.843		Crippen Method
mcvol	105.880	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	1017.00		NIST Webbook
rinpol	1049.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1061.00		NIST Webbook
tb	490.34	K	Joback Method
tc	717.23	K	Joback Method
tf	348.51	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.40	J/mol×K	490.34	Joback Method

cpg	233.90	J/mol×K	528.16	Joback Method
cpg	246.65	J/mol×K	565.97	Joback Method
cpg	258.67	J/mol×K	603.79	Joback Method
cpg	269.98	J/mol×K	641.60	Joback Method
cpg	280.60	J/mol×K	679.42	Joback Method
cpg	290.53	J/mol×K	717.23	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=C25343571&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