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

Inchi: InChI=1S/C7H11NO/c1-6(9)7-4-2-3-5-8-7/h2-5H2,1H3
InchiKey: GNZWXNKZMHJXNU-UHFFFAOYSA-N
Formula: C7H11NO
SMILES: CC(=O)C1=NCCCC1
Mol. weight [g/mol]: 125.17
CAS: 27300-27-2

Physical Properties

Property code	Value	Unit	Source
gf	48.41	kJ/mol	Joback Method
hf	-108.45	kJ/mol	Joback Method
hfus	12.22	kJ/mol	Joback Method
hvap	45.82	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.200		Crippen Method
mcvol	105.880	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
rinpol	1110.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1110.00		NIST Webbook
ripol	1619.00		NIST Webbook
ripol	1585.00		NIST Webbook
tb	495.49	K	Joback Method
tc	726.87	K	Joback Method
tf	315.02	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.69	J/mol×K	495.49	Joback Method
cpg	250.87	J/mol×K	534.05	Joback Method
cpg	265.18	J/mol×K	572.62	Joback Method
cpg	278.64	J/mol×K	611.18	Joback Method

cpg	291.26	J/mol×K	649.74	Joback Method
cpg	303.03	J/mol×K	688.31	Joback Method
cpg	313.98	J/mol×K	726.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27300272&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume