2-acetyl-3-ethylidene-3,4,5,6-tetrahydropyridine

Inchi: InChI=1S/C9H13NO/c1-3-8-5-4-6-10-9(8)7(2)11/h3H,4-6H2,1-2H3/b8-3+
InchiKey: GAEQLABCUJPAHA-FPYGCLRLSA-N
Formula: C9H13NO
SMILES: CC=C1CCCN=C1C(C)=O
Mol. weight [g/mol]: 151.21

Physical Properties

Property code	Value	Unit	Source
gf	110.71	kJ/mol	Joback Method
hf	-73.70	kJ/mol	Joback Method
hfus	17.72	kJ/mol	Joback Method
hvap	51.06	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.756		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
rinpol	1472.00		NIST Webbook
rinpol	1472.00		NIST Webbook
tb	547.89	K	Joback Method
tc	778.58	K	Joback Method
tf	347.92	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.89	J/mol×K	547.89	Joback Method
cpg	323.73	J/mol×K	586.34	Joback Method
cpg	338.62	J/mol×K	624.79	Joback Method
cpg	352.58	J/mol×K	663.23	Joback Method
cpg	365.63	J/mol×K	701.68	Joback Method
cpg	377.78	J/mol×K	740.13	Joback Method
cpg	389.04	J/mol×K	778.58	Joback Method

Sources

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=R231062&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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