2-acetyl-2-pyrroline

Inchi: InChI=1S/C6H9NO/c1-5(8)6-3-2-4-7-6/h3,7H,2,4H2,1H3
InchiKey: ZEKCQHIPQALHSP-UHFFFAOYSA-N
Formula: C6H9NO
SMILES: CC(=O)C1=CCCN1
Mol. weight [g/mol]: 111.14

Physical Properties

Property code	Value	Unit	Source
gf	23.02	kJ/mol	Joback Method
hf	-114.81	kJ/mol	Joback Method
hfus	16.18	kJ/mol	Joback Method
hvap	43.97	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	0.453		Crippen Method
mcvol	91.790	ml/mol	McGowan Method
pc	4615.13	kPa	Joback Method
rinpol	929.00		NIST Webbook
rinpol	916.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1327.00		NIST Webbook
tb	463.19	K	Joback Method
tc	684.93	K	Joback Method
tf	340.76	K	Joback Method
vc	0.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.23	J/mol×K	463.19	Joback Method
cpg	191.55	J/mol×K	500.15	Joback Method
cpg	202.24	J/mol×K	537.10	Joback Method
cpg	212.33	J/mol×K	574.06	Joback Method
cpg	221.83	J/mol×K	611.02	Joback Method
cpg	230.77	J/mol×K	647.98	Joback Method

cpg	239.16	J/mol×K	684.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R225968&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