2-Propionyl-1-pyrroline

Other names: 1-Pyrroline, 2-propanoyl
Inchi: InChI=1S/C7H11NO/c1-2-7(9)6-4-3-5-8-6/h2-5H2,1H3
InchiKey: OVNCGQSYSSYBPO-UHFFFAOYSA-N
Formula: C7H11NO
SMILES: CCC(=O)C1=NCCC1
Mol. weight [g/mol]: 125.17

Physical Properties

Property code	Value	Unit	Source
gf	60.51	kJ/mol	Joback Method
hf	-102.29	kJ/mol	Joback Method
hfus	14.32	kJ/mol	Joback Method
hvap	45.65	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.200		Crippen Method
mcvol	105.880	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
rinpol	1023.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1023.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1461.00		NIST Webbook
ripol	1427.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1445.00		NIST Webbook
ripol	1427.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1445.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1434.00		NIST Webbook
ripol	1413.00		NIST Webbook

ripol	1415.00		NIST Webbook
tb	491.22	K	Joback Method
tc	713.84	K	Joback Method
tf	318.54	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.14	J/mol×K	491.22	Joback Method
cpg	250.32	J/mol×K	528.32	Joback Method
cpg	263.70	J/mol×K	565.43	Joback Method
cpg	276.30	J/mol×K	602.53	Joback Method
cpg	288.13	J/mol×K	639.63	Joback Method
cpg	299.22	J/mol×K	676.73	Joback Method
cpg	309.58	J/mol×K	713.84	Joback Method

Sources

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=U298554&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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