

2-Acetyl-1-pyrroline

Other names:	1-Pyrroline, 2-acetyl 2-Acetyl-4,5-dihydro-3H-pyrrole 2-Acetyl-1-pyrroline
Inchi:	InChI=1S/C6H9NO/c1-5(8)6-3-2-4-7-6/h2-4H2,1H3
InchiKey:	DQBQWWSFRPLIAX-UHFFFAOYSA-N
Formula:	C6H9NO
SMILES:	CC(=O)C1=NCCC1
Mol. weight [g/mol]:	111.14
CAS:	85213-22-5

Physical Properties

Property code	Value	Unit	Source
gf	52.09	kJ/mol	Joback Method
hf	-81.65	kJ/mol	Joback Method
hfus	11.73	kJ/mol	Joback Method
hvap	43.43	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	0.810		Crippen Method
mcvol	91.790	ml/mol	McGowan Method
pc	4468.24	kPa	Joback Method
rinpol	924.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	892.00		NIST Webbook

rinpol	922.00	NIST Webbook
rinpol	922.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	922.00	NIST Webbook
rinpol	921.00	NIST Webbook
rinpol	898.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	925.00	NIST Webbook
rinpol	925.00	NIST Webbook
rinpol	892.00	NIST Webbook
rinpol	918.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	896.00	NIST Webbook
rinpol	920.00	NIST Webbook
rinpol	918.00	NIST Webbook
rinpol	921.00	NIST Webbook
rinpol	922.00	NIST Webbook
rinpol	928.00	NIST Webbook
rinpol	923.00	NIST Webbook
rinpol	923.00	NIST Webbook
rinpol	928.00	NIST Webbook
rinpol	926.00	NIST Webbook
rinpol	925.00	NIST Webbook
rinpol	922.00	NIST Webbook
rinpol	922.00	NIST Webbook
rinpol	917.00	NIST Webbook
rinpol	934.00	NIST Webbook
rinpol	921.00	NIST Webbook
rinpol	922.00	NIST Webbook
rinpol	924.00	NIST Webbook
rinpol	906.00	NIST Webbook
rinpol	921.00	NIST Webbook
rinpol	922.00	NIST Webbook
rinpol	918.00	NIST Webbook
rinpol	918.00	NIST Webbook
rinpol	922.00	NIST Webbook
rinpol	920.00	NIST Webbook
rinpol	922.00	NIST Webbook
rinpol	922.00	NIST Webbook
rinpol	916.00	NIST Webbook
rinpol	935.00	NIST Webbook
rinpol	935.00	NIST Webbook
rinpol	920.00	NIST Webbook

rinpol	927.00	NIST Webbook
rinpol	916.00	NIST Webbook
rinpol	921.00	NIST Webbook
rinpol	921.00	NIST Webbook
rinpol	919.00	NIST Webbook
rinpol	923.00	NIST Webbook
rinpol	925.00	NIST Webbook
rinpol	916.00	NIST Webbook
rinpol	921.00	NIST Webbook
rinpol	916.00	NIST Webbook
rinpol	925.00	NIST Webbook
rinpol	925.00	NIST Webbook
rinpol	922.00	NIST Webbook
rinpol	926.00	NIST Webbook
rinpol	920.00	NIST Webbook
rinpol	918.00	NIST Webbook
rinpol	926.00	NIST Webbook
rinpol	930.00	NIST Webbook
rinpol	928.00	NIST Webbook
rinpol	925.00	NIST Webbook
rinpol	929.00	NIST Webbook
rinpol	922.00	NIST Webbook
rinpol	922.00	NIST Webbook
rinpol	925.00	NIST Webbook
rinpol	930.00	NIST Webbook
rinpol	927.00	NIST Webbook
rinpol	912.00	NIST Webbook
ripol	1337.00	NIST Webbook
ripol	1340.00	NIST Webbook
ripol	1343.00	NIST Webbook
ripol	1314.00	NIST Webbook
ripol	1334.00	NIST Webbook
ripol	1323.00	NIST Webbook
ripol	1327.00	NIST Webbook
ripol	1328.00	NIST Webbook
ripol	1340.00	NIST Webbook
ripol	1335.00	NIST Webbook
ripol	1330.00	NIST Webbook
ripol	1326.00	NIST Webbook
ripol	1352.00	NIST Webbook
ripol	1317.00	NIST Webbook
ripol	1343.00	NIST Webbook
ripol	1319.00	NIST Webbook
ripol	1317.00	NIST Webbook

ripol	1309.00	NIST Webbook
ripol	1328.00	NIST Webbook
ripol	1328.00	NIST Webbook
ripol	1322.00	NIST Webbook
ripol	1323.00	NIST Webbook
ripol	1347.00	NIST Webbook
ripol	1348.00	NIST Webbook
ripol	1314.00	NIST Webbook
ripol	1335.00	NIST Webbook
ripol	1317.00	NIST Webbook
ripol	1335.00	NIST Webbook
ripol	1339.00	NIST Webbook
ripol	1337.00	NIST Webbook
ripol	1330.00	NIST Webbook
ripol	1341.00	NIST Webbook
ripol	1338.00	NIST Webbook
ripol	1338.00	NIST Webbook
ripol	1345.00	NIST Webbook
ripol	1326.00	NIST Webbook
ripol	1340.00	NIST Webbook
ripol	1377.00	NIST Webbook
ripol	1374.00	NIST Webbook
ripol	1374.00	NIST Webbook
ripol	1352.00	NIST Webbook
ripol	1345.00	NIST Webbook
ripol	1323.00	NIST Webbook
ripol	1327.00	NIST Webbook
ripol	1338.00	NIST Webbook
ripol	1317.00	NIST Webbook
ripol	1338.00	NIST Webbook
ripol	1323.00	NIST Webbook
ripol	1327.00	NIST Webbook
ripol	1327.00	NIST Webbook
ripol	1325.00	NIST Webbook
ripol	1355.00	NIST Webbook
ripol	1330.00	NIST Webbook
ripol	1330.00	NIST Webbook
ripol	1327.00	NIST Webbook
ripol	1328.00	NIST Webbook
ripol	1330.00	NIST Webbook
ripol	1330.00	NIST Webbook
ripol	1348.00	NIST Webbook
ripol	1322.00	NIST Webbook
ripol	1324.00	NIST Webbook

ripol	1328.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1329.00		NIST Webbook
ripol	1319.00		NIST Webbook
ripol	1326.00		NIST Webbook
ripol	1333.00		NIST Webbook
ripol	1333.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1311.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1317.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1340.00		NIST Webbook
ripol	1335.00		NIST Webbook
ripol	1319.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1335.00		NIST Webbook
ripol	1337.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1334.00		NIST Webbook
tb	468.34	K	Joback Method
tc	694.64	K	Joback Method
tf	307.27	K	Joback Method
vc	0.354	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.13	J/mol×K	468.34	Joback Method
cpg	207.13	J/mol×K	506.06	Joback Method
cpg	219.40	J/mol×K	543.77	Joback Method
cpg	230.97	J/mol×K	581.49	Joback Method
cpg	241.83	J/mol×K	619.20	Joback Method

cpg	252.00	J/mol×K	656.92	Joback Method
cpg	261.49	J/mol×K	694.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85213225&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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

Latest version available from:

<https://www.chemeo.com/cid/49-354-5/2-Acetyl-1-pyrroline.pdf>

Generated by Cheméo on 2024-04-25 03:36:16.730442129 +0000 UTC m=+16305425.651019444.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.