3-n-Propyl-2-pyrazolin-5-one

Other names: 3H-Pyrazol-3-one, 2,4-dihydro-5-propyl-
3-Propyl-2-pyrazolin-5-one
Inchi: InChI=1S/C6H10N2O/c1-2-3-5-4-6(9)8-7-5/h2-4H2,1H3,(H,8,9)
InchiKey: GVUNLYBSNQOHBD-UHFFFAOYSA-N
Formula: C6H10N2O
SMILES: CCCC1=NN=C(O)C1
Mol. weight [g/mol]: 126.16
CAS: 29211-70-9

Physical Properties

Property code	Value	Unit	Source
gf	181.30	kJ/mol	Joback Method
hf	-4.02	kJ/mol	Joback Method
hfus	20.19	kJ/mol	Joback Method
hvap	60.52	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.503		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	4789.21	kPa	Joback Method
tb	564.49	K	Joback Method
tc	777.25	K	Joback Method
tf	402.98	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.91	J/mol×K	564.49	Joback Method
cpg	275.83	J/mol×K	599.95	Joback Method
cpg	287.12	J/mol×K	635.41	Joback Method
cpg	297.77	J/mol×K	670.87	Joback Method
cpg	307.77	J/mol×K	706.33	Joback Method
cpg	317.11	J/mol×K	741.79	Joback Method
cpg	325.80	J/mol×K	777.25	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=C29211709&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume