

5-Amino-2-pyridone

Inchi:	InChI=1S/C5H6N2O/c6-4-1-2-5(8)7-3-4/h1,3H,2,6H2
InchiKey:	CHYPHWOOCGECMN-UHFFFAOYSA-N
Formula:	C5H6N2O
SMILES:	NC1=CCC(=O)N=C1
Mol. weight [g/mol]:	110.11
CAS:	33630-94-3

Physical Properties

Property code	Value	Unit	Source
gf	134.31	kJ/mol	Joback Method
hf	-0.72	kJ/mol	Joback Method
hfus	11.37	kJ/mol	Joback Method
hvap	49.81	kJ/mol	Joback Method
log10ws	-0.53		Crippen Method
logp	-0.170		Crippen Method
mcvol	83.380	ml/mol	McGowan Method
pc	5827.17	kPa	Joback Method
tb	535.37	K	Joback Method
tc	796.74	K	Joback Method
tf	394.79	K	Joback Method
vc	0.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.54	J/molxK	535.37	Joback Method
cpg	204.64	J/molxK	578.93	Joback Method
cpg	216.06	J/molxK	622.49	Joback Method
cpg	226.77	J/molxK	666.06	Joback Method
cpg	236.70	J/molxK	709.62	Joback Method
cpg	245.81	J/molxK	753.18	Joback Method
cpg	254.06	J/molxK	796.74	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33630943&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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