5-Amino-7-oxo-1,2,3,4,6-pentazaindene

Inchi: InChI=1S/C4H2N6O/c5-4-6-2-1(3(11)7-4)8-10-9-2/h(H2,5,7,11)
InchiKey: DIOJRWLGOYZDED-UHFFFAOYSA-N
Formula: C4H2N6O
SMILES: N=C1N=C(O)C2=NN=NC2=N1
Mol. weight [g/mol]: 150.10

Physical Properties

Property code	Value	Unit	Source
gf	798.84	kJ/mol	Joback Method
hf	608.17	kJ/mol	Joback Method
hvap	89.17	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	0.112		Crippen Method
mcvol	89.750	ml/mol	McGowan Method
tb	785.75	K	Joback Method
tf	725.94	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.09	J/mol×K	785.75	Joback Method
cpg	40.70	J/mol×K	100.12	Joback Method
cpg	40.70	J/mol×K	100.12	Joback Method
cpg	40.70	J/mol×K	100.12	Joback Method
cpg	40.70	J/mol×K	100.12	Joback Method
cpg	40.70	J/mol×K	100.12	Joback Method
cpg	40.70	J/mol×K	100.12	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002140&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
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point