3-Penten-2-one, 4-amino-

Other names: Acetylacetonamine
4-Amino-3-penten-2-one
Inchi: InChI=1S/C5H9NO/c1-4(6)3-5(2)7/h3H,6H2,1-2H3/b4-3+
InchiKey: OSLAYKKXCYSJSF-ONEGZZNKSA-N
Formula: C5H9NO
SMILES: CC(=O)C=C(C)N
Mol. weight [g/mol]: 99.13
CAS: 1118-66-7

Physical Properties

Property code	Value	Unit	Source
gf	0.42	kJ/mol	Joback Method
hf	-117.89	kJ/mol	Joback Method
hfus	14.39	kJ/mol	Joback Method
hvap	44.15	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	0.438		Crippen Method
mcvol	88.560	ml/mol	McGowan Method
pc	4322.57	kPa	Joback Method
tb	482.50 ± 0.50	K	NIST Webbook
tc	651.55	K	Joback Method
tf	260.26	K	Joback Method
vc	0.332	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.81	J/mol×K	444.24	Joback Method
cpg	181.96	J/mol×K	478.79	Joback Method
cpg	190.60	J/mol×K	513.34	Joback Method
cpg	198.74	J/mol×K	547.89	Joback Method
cpg	206.42	J/mol×K	582.44	Joback Method
cpg	213.65	J/mol×K	617.00	Joback Method
cpg	220.47	J/mol×K	651.55	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=C1118667&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