2-Pentanone, 4-amino-4-methyl-

Other names:	Diacetonamine
	4-Amino-4-methyl-2-pentanone
	4-amino-4-methylpentan-2-one
Inchi:	InChI=1S/C6H13NO/c1-5(8)4-6(2,3)7/h4,7H2,1-3H3
InchiKey:	CQTRUFMMCCOKTA-UHFFFAOYSA-N
Formula:	C6H13NO
SMILES:	CC(=O)CC(C)(C)N
Mol. weight [g/mol]:	115.17
CAS:	625-04-7

Physical Properties

Property code	Value	Unit	Source
gf	-59.99	kJ/mol	Joback Method
hf	-254.71	kJ/mol	Joback Method
hfus	10.68	kJ/mol	Joback Method
hvap	45.04	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	0.703		Crippen Method
mcvol	106.950	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	452.50 ± 1.50	K	NIST Webbook
tc	663.86	K	Joback Method
tf	292.99	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.63	J/mol×K	459.85	Joback Method
cpg	243.50	J/mol×K	493.85	Joback Method
cpg	254.68	J/mol×K	527.85	Joback Method
cpg	265.19	J/mol×K	561.86	Joback Method
cpg	275.07	J/mol×K	595.86	Joback Method
cpg	284.34	J/mol×K	629.86	Joback Method

cpg	293.06	J/mol×K	663.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	298.00	K	0.03	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C625047&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
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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