ACETAMIDE, N-ACETYL-

Other names:	CH3C(O)NHC(O)CH3
	Bisacetylamine
	Acetamide, N-acetyl-
	Dicetylamine
	N-Acetylacetamide
	Diacetylamine
Inchi:	InChI=1S/C4H7NO2/c1-3(6)5-4(2)7/h1-2H3,(H,5,6,7)
InchiKey:	ZSBDPRIWBYHIAF-UHFFFAOYSA-N
Formula:	C4H7NO2
SMILES:	CC(=O)NC(C)=O
Mol. weight [g/mol]:	101.10

Physical Properties

Property code	Value	Unit	Source
af	0.4896		Cheméo Relay (1.0)
chs	-2087.52	kJ/mol	NIST Webbook
gf	-185.65	kJ/mol	Joback Method
hf	-474.08	kJ/mol	Cheméo Relay (1.0)
hfs	-500.80	kJ/mol	NIST Webbook
hfus	14.41	kJ/mol	Joback Method
hsub	73.20 ± 0.80	kJ/mol	NIST Webbook
hsub	73.20 ± 0.80	kJ/mol	NIST Webbook
hvap	49.61	kJ/mol	Cheméo Relay (1.0)
ie	9.55	eV	Cheméo Relay (1.0)
log10ws	0.21		Cheméo Relay (1.0)
logp	-0.331		Crippen Method
mcvol	80.340	ml/mol	McGowan Method
pc	4672.09	kPa	Joback Method
tb	496.70	K	NIST Webbook
tc	653.15	K	Cheméo Relay (1.0)
tf	356.45	K	Cheméo Relay (1.0)
vc	0.301	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.41	J/mol×K	448.83	Joback Method
cpg	163.03	J/mol×K	481.64	Joback Method
cpg	170.29	J/mol×K	514.44	Joback Method
cpg	177.20	J/mol×K	547.25	Joback Method
cpg	183.77	J/mol×K	580.05	Joback Method
cpg	190.02	J/mol×K	612.86	Joback Method
cpg	195.93	J/mol×K	645.66	Joback Method
hvapt	59.70	kJ/mol	432.00	NIST Webbook
hvapt	64.60	kJ/mol	419.50	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C625774&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hsub: Enthalpy of sublimation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

hvapt: Enthalpy of vaporization at a given temperature

ie: Ionization energy

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