Diacetamide

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
CAS:	625-77-4

Physical Properties

Property code	Value	Unit	Source
chs	-2087.52	kJ/mol	NIST Webbook
gf	-185.65	kJ/mol	Joback Method
hf	-297.58	kJ/mol	Joback Method
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	44.43	kJ/mol	Joback Method
log10ws	-0.24		Crippen Method
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	645.66	K	Joback Method
tf	287.36	K	Joback Method
vc	0.306	m3/kmol	Joback Method

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

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=C625774&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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