N-Methyldiacetamide

Other names: Diacetamide, N-methyl-
N-Methyldiacetamide
N,N-Diacetylmethylamine
N-Methyl-N-acetylacetamide
N-acetyl-N-methylacetamide
Inchi: InChI=1S/C5H9NO2/c1-4(7)6(3)5(2)8/h1-3H3
InchiKey: ZNQFZPCFVNOXJQ-UHFFFAOYSA-N
Formula: C5H9NO2
SMILES: CC(=O)N(C)C(C)=O
Mol. weight [g/mol]: 115.13

Physical Properties

Property code	Value	Unit	Source
af	0.4450		Cheméo Relay (1.0)
gf	-155.84	kJ/mol	Joback Method
hf	-445.25	kJ/mol	Cheméo Relay (1.0)
hfus	14.92	kJ/mol	Joback Method
hvap	53.47	kJ/mol	Cheméo Relay (1.0)
ie	9.65	eV	Cheméo Relay (1.0)
log10ws	0.64		Cheméo Relay (1.0)
logp	0.011		Crippen Method
mcvol	94.430	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
tb	466.00 ± 1.00	K	NIST Webbook
tc	635.42	K	Cheméo Relay (1.0)
tf	346.36	K	Cheméo Relay (1.0)
vc	0.362	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.27	J/mol×K	433.98	Joback Method
cpg	193.64	J/mol×K	465.54	Joback Method
cpg	202.56	J/mol×K	497.11	Joback Method

cpg	211.03	J/mol×K	528.67	Joback Method
cpg	219.07	J/mol×K	560.24	Joback Method
cpg	226.69	J/mol×K	591.80	Joback Method
cpg	233.91	J/mol×K	623.37	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1113684&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
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