

1-Acetyl-3-methylurea

Other names:	Acetamide, N-((methylamino)carbonyl)- N-Methyl-N'-acetylurea N'-Methyl-N-acetylurea Urea, 1-acetyl-3-methyl- Acetyl methyl urea
Inchi:	InChI=1S/C4H8N2O2/c1-3(7)6-4(8)5-2/h1-2H3,(H2,5,6,7,8)
InchiKey:	XRVHSOXXNQTWAW-UHFFFAOYSA-N
Formula:	C4H8N2O2
SMILES:	CNC(=O)NC(C)=O
Mol. weight [g/mol]:	116.12
CAS:	623-59-6

Physical Properties

Property code	Value	Unit	Source
chs	-2154.30 ± 2.30	kJ/mol	NIST Webbook
gf	-96.26	kJ/mol	Joback Method
hf	-244.11	kJ/mol	Joback Method
hfs	-563.10 ± 2.30	kJ/mol	NIST Webbook
hfus	19.51	kJ/mol	Joback Method
hvap	50.86	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	-0.538		Crippen Method
mvol	90.320	ml/mol	McGowan Method
pc	4756.24	kPa	Joback Method
tb	499.00	K	Joback Method
tc	698.04	K	Joback Method
tf	340.02	K	Joback Method
vc	0.342	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.93	J/mol×K	499.00	Joback Method
cpg	201.23	J/mol×K	532.17	Joback Method

cpg	209.10	J/mol×K	565.35	Joback Method
cpg	216.57	J/mol×K	598.52	Joback Method
cpg	223.63	J/mol×K	631.70	Joback Method
cpg	230.30	J/mol×K	664.87	Joback Method
cpg	236.58	J/mol×K	698.04	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C623596&Units=SI

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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