

Ethanone, 1-(4,5-dihydro-2-thiazolyl)-

Other names:	2-Acetyl-2-thiazoline 1-(4,5-Dihydro-1,3-thiazol-2-yl)ethanone 2-Acetylthiazoline 2-Thiazoline, 2-acetyl Ketone, methyl 2-thiazolin-2-yl Acetylthiazoline
Inchi:	InChI=1S/C5H7NOS/c1-4(7)5-6-2-3-8-5/h2-3H2,1H3
InchiKey:	FZOZFDAMVVEZSJ-UHFFFAOYSA-N
Formula:	C5H7NOS
SMILES:	CC(=O)C1=NCCS1
Mol. weight [g/mol]:	129.18
CAS:	29926-41-8

Physical Properties

Property code	Value	Unit	Source
gf	83.53	kJ/mol	Joback Method
hf	-15.75	kJ/mol	Joback Method
hfus	12.80	kJ/mol	Joback Method
hvap	47.01	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.721		Crippen Method
mcvol	94.050	ml/mol	McGowan Method
pc	5058.59	kPa	Joback Method
rinpol	1105.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1105.00		NIST Webbook
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rinpol	1063.00		NIST Webbook

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rinpol	1111.00	NIST Webbook
rinpol	1106.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1111.00	NIST Webbook
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ripol	1728.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1755.00		NIST Webbook
tb	493.29	K	Joback Method
tc	738.41	K	Joback Method
tf	379.45	K	Joback Method
vc	0.344	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.10	J/molxK	493.29	Joback Method
cpg	205.74	J/molxK	534.14	Joback Method
cpg	216.63	J/molxK	575.00	Joback Method
cpg	226.80	J/molxK	615.85	Joback Method
cpg	236.26	J/molxK	656.70	Joback Method
cpg	245.03	J/molxK	697.56	Joback Method
cpg	253.11	J/molxK	738.41	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=C29926418&Units=SI>

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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinp:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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