

# 2,4-Thiazolidinedione, 5-isopropylidene

<b>Inchi:</b>	InChI=1S/C6H7NO2S/c1-3(2)4-5(8)7-6(9)10-4/h1-2H3,(H,7,8,9)
<b>InchiKey:</b>	QOWVABKYNPDNIM-UHFFFAOYSA-N
<b>Formula:</b>	C6H7NO2S
<b>SMILES:</b>	CC(C)=C1SC(=O)NC1=O
<b>Mol. weight [g/mol]:</b>	157.19
<b>CAS:</b>	5835-47-2

## Physical Properties

Property code	Value	Unit	Source
gf	-36.80	kJ/mol	Joback Method
hf	-212.44	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	51.45	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.263		Crippen Method
mcvol	109.710	ml/mol	McGowan Method
pc	4704.19	kPa	Joback Method
tb	595.17	K	Joback Method
tc	863.01	K	Joback Method
tf	493.84	K	Joback Method
vc	0.395	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.70	J/molxK	595.17	Joback Method
cpg	256.89	J/molxK	639.81	Joback Method
cpg	268.47	J/molxK	684.45	Joback Method
cpg	279.35	J/molxK	729.09	Joback Method
cpg	289.49	J/molxK	773.73	Joback Method
cpg	298.82	J/molxK	818.37	Joback Method
cpg	307.27	J/molxK	863.01	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5835472&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5835472&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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