

# 9,10-Anthracenedione, 1-methyl-

<b>Other names:</b>	Anthraquinone, 1-methyl- «alpha»-Methylantraquinone 1-Methyl-9,10-anthraquinone 1-Methylantraquinone Antracene-9,10(9H,10H)-dione, 1-methyl- 1-Methylantracenedione
<b>Inchi:</b>	InChI=1S/C15H10O2/c1-9-5-4-8-12-13(9)15(17)11-7-3-2-6-10(11)14(12)16/h2-8H,1H3
<b>InchiKey:</b>	RBGUKBSLNOTVCD-UHFFFAOYSA-N
<b>Formula:</b>	C15H10O2
<b>SMILES:</b>	<chem>Cc1cccc2c1C(=O)c1cccc1C2=O</chem>
<b>Mol. weight [g/mol]:</b>	222.24
<b>CAS:</b>	954-07-4

## Physical Properties

Property code	Value	Unit	Source
gf	106.73	kJ/mol	Joback Method
hf	-90.38	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	64.07	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	2.770		Crippen Method
mvol	166.970	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	344.50		NIST Webbook
tb	753.68	K	Joback Method
tc	1022.79	K	Joback Method
tf	511.35	K	Joback Method
vc	0.639	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.00	J/mol×K	753.68	Joback Method
cpg	466.44	J/mol×K	798.53	Joback Method

cpg	479.63	J/mol×K	843.38	Joback Method
cpg	491.63	J/mol×K	888.23	Joback Method
cpg	502.47	J/mol×K	933.09	Joback Method
cpg	512.19	J/mol×K	977.94	Joback Method
cpg	520.84	J/mol×K	1022.79	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=C954074&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C954074&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>rinpola:</b>	Non-polar retention indices
<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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