

# 1,5-Dicarbomethoxy quadricyclane

<b>Inchi:</b>	InChI=1S/C11H12O4/c1-14-8(12)10-4-3-5-7(6(4)10)11(5,10)9(13)15-2/h4-7H,3H2,1-2H3
<b>InchiKey:</b>	JEA AFLQGDKNDNL-UHFFFAOYSA-N
<b>Formula:</b>	C11H12O4
<b>SMILES:</b>	COC(=O)C12C3CC4C(C31)C42C(=O)OC
<b>Mol. weight [g/mol]:</b>	208.21
<b>CAS:</b>	714-53-4

## Physical Properties

Property code	Value	Unit	Source
gf	-149.00	kJ/mol	Joback Method
hf	-448.17	kJ/mol	Joback Method
hfus	22.41	kJ/mol	Joback Method
hvap	54.26	kJ/mol	Joback Method
log10ws	-0.28		Crippen Method
logp	0.214		Crippen Method
mcvol	137.290	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
tb	600.41	K	Joback Method
tc	811.58	K	Joback Method
tf	486.73	K	Joback Method
vc	0.561	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.84	J/molxK	600.41	Joback Method
cpg	411.81	J/molxK	635.61	Joback Method
cpg	422.97	J/molxK	670.80	Joback Method
cpg	433.60	J/molxK	706.00	Joback Method
cpg	443.99	J/molxK	741.19	Joback Method
cpg	454.42	J/molxK	776.39	Joback Method
cpg	465.17	J/molxK	811.58	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=C714534&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C714534&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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