

# Dibenzo[def,mno]chrysene-6,12-dione

<b>Other names:</b>	Anthanthron Anthanthrone Helanthrene Orange GK Anthranthrone
<b>Inchi:</b>	InChI=1S/C22H10O2/c23-21-13-5-1-3-11-7-9-16-19(17(11)13)20-15(21)10-8-12-4-2-6-14
<b>InchiKey:</b>	PGEHNUUBUQTUJB-UHFFFAOYSA-N
<b>Formula:</b>	C22H10O2
<b>SMILES:</b>	O=c1c2ccc3cccc4c(=O)c5ccc6cccc1c6c5-c2c34
<b>Mol. weight [g/mol]:</b>	306.31
<b>CAS:</b>	641-13-4

## Physical Properties

Property code	Value	Unit	Source
ie	8.00	eV	NIST Webbook
log10ws	-7.80		Crippen Method
logp	4.438		Crippen Method
mvol	215.820	ml/mol	McGowan Method
rinpol	550.62		NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	152.20	kJ/mol	500.00	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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=C641134&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C641134&amp;Units=SI</a>

# Legend

<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>ie:</b>	Ionization energy
<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>rinpol:</b>	Non-polar retention indices

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