

# 2,2',2'',2''',4,4',4'',4''',6,6',6'',6'''-Dodecanitroquatrap

<b>Inchi:</b>	InChI=1S/C24H6N12O24/c37-25(38)7-1-9(27(41)42)17(10(2-7)28(43)44)19-13(31(49)50
<b>InchiKey:</b>	IFPMZBBHBZQTOV-UHFFFAOYSA-N
<b>Formula:</b>	C24H6N12O24
<b>SMILES:</b>	O=[N+]([O-])c1cc([N+](=O)[O-])c(-c2c([N+](=O)[O-])cc([N+](=O)[O-])c(-c3c([N+](=O)[O-])c
<b>Mol. weight [g/mol]:</b>	846.37
<b>CAS:</b>	23242-92-4

## Physical Properties

Property code	Value	Unit	Source
chs	-10515.00 ± 4.00	kJ/mol	NIST Webbook
gf	892.62	kJ/mol	Joback Method
hf	117.73	kJ/mol	Joback Method
hfs	213.00 ± 10.00	kJ/mol	NIST Webbook
hfus	164.97	kJ/mol	Joback Method
hvap	286.48	kJ/mol	Joback Method
log10ws	-17.09		Crippen Method
logp	5.586		Crippen Method
mcvol	463.020	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
tb	2747.04	K	Joback Method
tc	3950.56	K	Joback Method
tf	2364.52	K	Joback Method
vc	1.931	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1375.58	J/molxK	2747.04	Joback Method
cpg	1528.50	J/molxK	2947.63	Joback Method
cpg	1756.90	J/molxK	3148.21	Joback Method
cpg	2073.64	J/molxK	3348.80	Joback Method
cpg	2491.58	J/molxK	3549.39	Joback Method
cpg	3023.55	J/molxK	3749.98	Joback Method
cpg	3682.42	J/molxK	3950.56	Joback Method

# 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>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=C23242924&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23242924&amp;Units=SI</a>

# Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<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>hfs:</b>	Solid phase 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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