

# Decan-2-yl 3,5-dinitrobenzoate

<b>Inchi:</b>	InChI=1S/C17H24N2O6/c1-3-4-5-6-7-8-9-13(2)25-17(20)14-10-15(18(21)22)12-16(11-14
<b>InchiKey:</b>	HPYNBZPBELXXHU-UHFFFAOYSA-N
<b>Formula:</b>	C17H24N2O6
<b>SMILES:</b>	CCCCCCCCC(C)OC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	352.38

## Physical Properties

Property code	Value	Unit	Source
gf	20.15	kJ/mol	Joback Method
hf	-452.22	kJ/mol	Joback Method
hfus	55.03	kJ/mol	Joback Method
hvap	98.99	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	4.799		Crippen Method
mvol	268.910	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	2532.00		NIST Webbook
tb	1004.53	K	Joback Method
tc	1243.83	K	Joback Method
tf	677.19	K	Joback Method
vc	1.062	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.65	J/mol×K	1004.53	Joback Method
cpg	884.99	J/mol×K	1044.41	Joback Method
cpg	895.11	J/mol×K	1084.30	Joback Method
cpg	904.07	J/mol×K	1124.18	Joback Method
cpg	911.91	J/mol×K	1164.06	Joback Method
cpg	918.70	J/mol×K	1203.95	Joback Method
cpg	924.48	J/mol×K	1243.83	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=U373870&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U373870&amp;Units=SI</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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