

# Fumaric acid, 2-nitrophenyl naphth-2-ylmethyl ester

<b>Inchi:</b>	InChI=1S/C21H15NO6/c23-20(27-14-15-9-10-16-5-1-2-6-17(16)13-15)11-12-21(24)28-19
<b>InchiKey:</b>	KYXJFWKMIHDPSS-VAWYXSNFSA-N
<b>Formula:</b>	C21H15NO6
<b>SMILES:</b>	O=C(C=CC(=O)Oc1cccc1[N+](=O)[O-])OCc1ccc2ccccc2c1
<b>Mol. weight [g/mol]:</b>	377.35

## Physical Properties

Property code	Value	Unit	Source
gf	86.08	kJ/mol	Joback Method
hf	-218.72	kJ/mol	Joback Method
hfus	51.61	kJ/mol	Joback Method
hvap	104.72	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	3.953		Crippen Method
mvol	267.770	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	3201.00		NIST Webbook
rinpol	3201.00		NIST Webbook
tb	1070.76	K	Joback Method
tc	1335.57	K	Joback Method
tf	719.86	K	Joback Method
vc	1.028	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.75	J/molxK	1070.76	Joback Method
cpg	826.21	J/molxK	1114.89	Joback Method
cpg	834.82	J/molxK	1159.03	Joback Method
cpg	842.73	J/molxK	1203.16	Joback Method
cpg	850.08	J/molxK	1247.30	Joback Method
cpg	856.99	J/molxK	1291.43	Joback Method
cpg	863.59	J/molxK	1335.57	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=U405802&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405802&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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