

# (Z)-3-(o-Methylphenylamino)-2-nitrocrotonic acid methyl ester

Inchi:	InChI=1S/C12H14N2O4/c1-8-6-4-5-7-10(8)13-9(2)11(14(16)17)12(15)18-3/h4-7,13H,1-3
InchiKey:	BADBMFQWMIQDHO-LUAWRHEFSA-N
Formula:	C12H14N2O4
SMILES:	COC(=O)C(=C(C)Nc1cccc1C)[N+](=O)[O-]
Mol. weight [g/mol]:	250.25
CAS:	127727-81-5

## Physical Properties

Property code	Value	Unit	Source
gf	107.08	kJ/mol	Joback Method
hf	-170.40	kJ/mol	Joback Method
hfus	37.32	kJ/mol	Joback Method
hvap	77.55	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.088		Crippen Method
mcvol	186.720	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
tb	787.84	K	Joback Method
tc	1029.73	K	Joback Method
tf	499.37	K	Joback Method
vc	0.723	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.97	J/molxK	787.84	Joback Method
cpg	534.30	J/molxK	828.15	Joback Method
cpg	545.63	J/molxK	868.47	Joback Method
cpg	556.02	J/molxK	908.78	Joback Method
cpg	565.53	J/molxK	949.10	Joback Method
cpg	574.22	J/molxK	989.41	Joback Method
cpg	582.14	J/molxK	1029.73	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C127727815&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C127727815&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>
<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>

# 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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