

# bis-(3-Nitrophenyl)acetic acid, methyl ester

<b>Inchi:</b>	InChI=1S/C15H12N2O6/c1-23-15(18)14(10-4-2-6-12(8-10)16(19)20)11-5-3-7-13(9-11)17
<b>InchiKey:</b>	BXQDHYSPLQKDRU-UHFFFAOYSA-N
<b>Formula:</b>	C15H12N2O6
<b>SMILES:</b>	COC(=O)C(c1cccc([N+](=O)[O-])c1)c1cccc([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	316.27

## Physical Properties

Property code	Value	Unit	Source
gf	115.72	kJ/mol	Joback Method
hf	-174.41	kJ/mol	Joback Method
hfus	43.90	kJ/mol	Joback Method
hvap	96.81	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	2.808		Crippen Method
mvol	216.970	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	2583.00		NIST Webbook
rinpol	2583.00		NIST Webbook
tb	985.45	K	Joback Method
tc	1260.43	K	Joback Method
tf	681.07	K	Joback Method
vc	0.842	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.67	J/mol×K	985.45	Joback Method
cpg	656.37	J/mol×K	1031.28	Joback Method
cpg	663.79	J/mol×K	1077.11	Joback Method
cpg	670.00	J/mol×K	1122.94	Joback Method
cpg	675.09	J/mol×K	1168.77	Joback Method
cpg	679.15	J/mol×K	1214.60	Joback Method
cpg	682.25	J/mol×K	1260.43	Joback Method

# Sources

<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=R190040&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R190040&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>

# 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>hvp:</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>rinp:</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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