

# 2,Beta-dinitrostyrene

<b>Inchi:</b>	InChI=1S/C8H6N2O4/c11-9(12)6-5-7-3-1-2-4-8(7)10(13)14/h1-6H/b6-5+
<b>InchiKey:</b>	INIQBBVYBCGEIX-AATRIKPKSA-N
<b>Formula:</b>	C8H6N2O4
<b>SMILES:</b>	O=[N+]([O-])C=Cc1ccccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	194.14
<b>CAS:</b>	3156-39-6

## Physical Properties

Property code	Value	Unit	Source
gf	270.58	kJ/mol	Joback Method
hf	112.31	kJ/mol	Joback Method
hfus	33.05	kJ/mol	Joback Method
hvap	69.48	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	1.842		Crippen Method
mcvol	130.360	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	721.94	K	Joback Method
tc	999.91	K	Joback Method
tf	501.00	K	Joback Method
vc	0.519	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.64	J/molxK	721.94	Joback Method
cpg	335.45	J/molxK	768.27	Joback Method
cpg	344.32	J/molxK	814.60	Joback Method
cpg	352.34	J/molxK	860.93	Joback Method
cpg	359.62	J/molxK	907.25	Joback Method
cpg	366.26	J/molxK	953.58	Joback Method
cpg	372.36	J/molxK	999.91	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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=C3156396&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3156396&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>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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