

# N-(2,3-dichlorophenyl)-n-[(e)-(3-nitrophenyl)methyl]

**Inchi:** InChI=1S/C13H8Cl2N2O2/c14-11-5-2-6-12(13(11)15)16-8-9-3-1-4-10(7-9)17(18)19/h1-8  
**InchiKey:** XTJVPSSTGZWXLC-LZYBPNLTSA-N  
**Formula:** C13H8Cl2N2O2  
**SMILES:** O=[N+]([O-])c1cccc(C=Nc2cccc(Cl)c2Cl)c1  
**Mol. weight [g/mol]:** 295.12  
**CAS:** 116465-42-0

## Physical Properties

Property code	Value	Unit	Source
hf	166.98	kJ/mol	Joback Method
hvap	79.74	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.652		Crippen Method
mcvol	194.090	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
tb	868.52	K	Joback Method
tc	1151.80	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C116465420&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** 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

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