

# Ether, 2,4-dibromophenyl p-nitrophenyl-

<b>Other names:</b>	Ether, 2,6-dichlorophenyl p-nitrophenyl-,
<b>Inchi:</b>	InChI=1S/C12H7Cl2NO3/c13-10-2-1-3-11(14)12(10)18-9-6-4-8(5-7-9)15(16)17/h1-7H
<b>InchiKey:</b>	NCCRTWSKGUMZTF-UHFFFAOYSA-N
<b>Formula:</b>	C12H7Cl2NO3
<b>SMILES:</b>	O=[N+]([O-])c1ccc(Oc2c(Cl)cccc2Cl)cc1
<b>Mol. weight [g/mol]:</b>	284.10
<b>CAS:</b>	2093-28-9

## Physical Properties

Property code	Value	Unit	Source
gf	152.78	kJ/mol	Joback Method
hf	-26.82	kJ/mol	Joback Method
hfus	34.69	kJ/mol	Joback Method
hvap	76.61	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.694		Crippen Method
mcvol	180.190	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
tb	791.38	K	Joback Method
tc	1065.45	K	Joback Method
tf	541.08	K	Joback Method
vc	0.690	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.12	J/molxK	791.38	Joback Method
cpg	445.46	J/molxK	837.06	Joback Method
cpg	454.67	J/molxK	882.74	Joback Method
cpg	462.81	J/molxK	928.41	Joback Method
cpg	469.92	J/molxK	974.09	Joback Method
cpg	476.06	J/molxK	1019.77	Joback Method
cpg	481.28	J/molxK	1065.45	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C2093289&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2093289&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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