

# 1-Amino-2-bromo-4-p-toluidinoanthraquinone

<b>Other names:</b>	1-Amino-2-bromo-4-[(4-methylphenyl)amino]-9,10-anthraquinone
<b>Inchi:</b>	InChI=1S/C21H15BrN2O2/c1-11-6-8-12(9-7-11)24-16-10-15(22)19(23)18-17(16)20(25)1
<b>InchiKey:</b>	SPDRRRCQUXHHLH-UHFFFAOYSA-N
<b>Formula:</b>	C21H15BrN2O2
<b>SMILES:</b>	<chem>Cc1ccc(Nc2cc(Br)c(N)c3c2C(=O)c2cccc2C3=O)cc1</chem>
<b>Mol. weight [g/mol]:</b>	407.26
<b>CAS:</b>	128-83-6

## Physical Properties

Property code	Value	Unit	Source
gf	410.93	kJ/mol	Joback Method
hf	101.49	kJ/mol	Joback Method
hfus	43.70	kJ/mol	Joback Method
hvap	105.20	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	4.859		Crippen Method
mcvol	265.210	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
tb	1121.44	K	Joback Method
tc	1407.71	K	Joback Method
tf	838.67	K	Joback Method
vc	0.994	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.99	J/molxK	1121.44	Joback Method
cpg	817.77	J/molxK	1169.15	Joback Method
cpg	825.30	J/molxK	1216.86	Joback Method
cpg	831.70	J/molxK	1264.57	Joback Method
cpg	837.07	J/molxK	1312.29	Joback Method
cpg	841.49	J/molxK	1360.00	Joback Method
cpg	845.08	J/molxK	1407.71	Joback Method
hsubt	167.00 ± 6.00	kJ/mol	428.00	NIST Webbook

# 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.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=C128836&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C128836&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>hsub:</b>	Enthalpy of sublimation at a given temperature
<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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