

# Solvent blue 35,CI 61554

<b>Other names:</b>	9,10-Anthracenedione, 1,4-bis(butylamino)- 1,4-bis(butylamino)anthraquinone 1,4-bis(N-butylamino)-9,10-anthraquinone
<b>Inchi:</b>	InChI=1S/C22H26N2O2/c1-3-5-13-23-17-11-12-18(24-14-6-4-2)20-19(17)21(25)15-9-7-8
<b>InchiKey:</b>	OCQDPIXQTSYZJL-UHFFFAOYSA-N
<b>Formula:</b>	C22H26N2O2
<b>SMILES:</b>	CCCCNc1ccc(NCCCC)c2c1C(=O)c1cccc1C2=O
<b>Mol. weight [g/mol]:</b>	350.45
<b>CAS:</b>	17354-14-2

## Physical Properties

Property code	Value	Unit	Source
gf	334.82	kJ/mol	Joback Method
hf	-139.39	kJ/mol	Joback Method
hfus	47.64	kJ/mol	Joback Method
hvap	93.18	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	4.886		Crippen Method
mcvol	285.560	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
tb	1019.16	K	Joback Method
tc	1260.26	K	Joback Method
tf	708.08	K	Joback Method
vc	1.101	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.33	J/molxK	1019.16	Joback Method
cpg	968.74	J/molxK	1059.34	Joback Method
cpg	980.84	J/molxK	1099.53	Joback Method
cpg	991.68	J/molxK	1139.71	Joback Method
cpg	1001.32	J/molxK	1179.90	Joback Method
cpg	1009.83	J/molxK	1220.08	Joback Method

cpg	1017.25	J/mol×K	1260.26	Joback Method
hsubt	116.40 ± 2.30	kJ/mol	393.50	NIST Webbook

## 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=C17354142&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17354142&amp;Units=SI</a>
<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>

## 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>hsubt:</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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