9,10-Anthracenedione, 1-(methylamino)-4-[(4-methylphenyl)amino]-

Other names: Ahcoquinone Blue ASTB Base
Alizarine Pure Blue B Base
Anthraquinone, 1-(methylamino)-4-p-toluidino-
C.I. Solvent Blue 11
C.I. 61525
Nitro Fast Blue 3GB
Organol Blue J
Organol Brilliant Blue J
Solvent Blue 11
Somalia Blue G
Sudan Blue GA
Superlan Astrol B Base
Waxoline Blue GA
1-(Methylamino)-4-p-toluidinoanthraquinone
1-Methylamino-4-(4-methylphenylamino)anthraquinone
NSC 39906
1-(N-methylamino)-4-[(4-methylphenyl)amino]-9,10-anthraquinone

Inchi: InChI=1S/C22H18N2O2/c1-13-7-9-14(10-8-13)24-18-12-11-17(23-2)19-20(18)22(26)16-6

InchiKey: ITYXXSSJBOAGAR-UHFFFAOYSA-N

Formula: C22H18N2O2

SMILES: CNc1ccc(Nc2ccc(C)cc2)c2c1C(=O)c1ccccc1C2=O

Mol. weight [g/mol]: 342.39

CAS: 128-85-8

Physical Properties

Property code	Value	Unit	Source
gf	437.60	kJ/mol	Joback Method
hf	85.67	kJ/mol	Joback Method
hfus	41.30	kJ/mol	Joback Method
hvap	96.12	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.556		Crippen Method
mcvol	261.800	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
tb	1050.82	K	Joback Method
tc	1319.11	K	Joback Method
tf	747.02	K	Joback Method

vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.24	J/mol×K	1050.82	Joback Method
cpg	852.27	J/mol×K	1095.53	Joback Method
cpg	861.89	J/mol×K	1140.25	Joback Method
cpg	870.17	J/mol×K	1184.96	Joback Method
cpg	877.21	J/mol×K	1229.68	Joback Method
cpg	883.09	J/mol×K	1274.39	Joback Method
cpg	887.89	J/mol×K	1319.11	Joback Method
hsubt	153.90 ± 3.90	kJ/mol	414.50	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C128858&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume