SUDAN BLUE

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]:	342.40

Physical Properties

Property code	Value	Unit	Source
hfus	41.30	kJ/mol	Joback Method
logp	4.556		Crippen Method
mcvol	261.800	ml/mol	McGowan 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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C128858&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume