Disperse Blue 1

Other names:

9,10-Anthracenedione, 1,4,5,8-tetraamino-
Acetate Blue G
Acetoquinone Blue L
Acetoquinone Blue R
Acetylon Fast Blue G
Amacel Blue GG
Amacel Pure Blue B
Anthraquinone, 1,4,5,8-tetraamino-
Artisil Blue SAP
Artisil Blue SAP Conc
Brasilazet Blue GR
C.I. Disperse Blue 1
C.I. Solvent Blue 18
C.I. 64500
Celanthrene Pure Blue BRS
Celliton Blue BB-CF
Celliton Blue Extra
Celliton Blue G
Celliton Blue GA-CF
Cibacet Sapphire Blue G
Cibacete Sapphire Blue G
Cilla Blue Extra
Diacelliton Fast Blue R
Disperse Blue NO 1
Duranol Brilliant Blue CB
Fenacet Blue G
Grasol Blue 2GS
Kayalon Fast Blue BR
Microsetile Blue EB
Miketon Fast Blue
Miketon Fast Blue B
Nacelan Blue G
Neosetile Blue EB
Nyloquinone Blue 2J
NCI-C54900
Oracet Sapphire Blue G
Perliton Blue B
Serinyl Blue 2G
Serinyl Blue 3G
Serinyl Blue 3GN

	Setacyl Blue 2GS
	Setacyl Blue 2GS II
	Solvent Blue 18
	Supracet Brilliant Blue 2GN
	Supracet Deep Blue R
	1,4,5,8-Tetraamino-9,10-anthracenedione
	1,4,5,8-Tetraaminoanthraquinone
	1,4,5,8-Tetraminoanthraquinone
	Anthraquinone, 1,4,5,8-tetramino-
	NSC 39936
Inchi:	InChI=1S/C14H12N4O2/c15-5-1-2-6(16)10-9(5)13(19)11-7(17)3-4-8(18)12(11)14(10)20/h
InchiKey:	JSFUMBWFPQSADC-UHFFFAOYSA-N
Formula:	C14H12N4O2
SMILES:	Nc1ccc(N)c2c1C(=O)c1c(N)ccc(N)c1C2=O
Mol. weight [g/mol]:	268.27
CAS:	2475-45-8

Physical Properties

Property code	Value	Unit	Source
gf	335.22	kJ/mol	Joback Method
hf	31.01	kJ/mol	Joback Method
hfus	36.74	kJ/mol	Joback Method
hvap	106.39	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	0.791		Crippen Method
mcvol	192.800	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
tb	1035.86	K	Joback Method
tc	1321.36	K	Joback Method
tf	870.68	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.64	J/mol×K	1035.86	Joback Method
cpg	614.57	J/mol×K	1083.44	Joback Method

cpg	621.14	J/mol×K	1131.03	Joback Method
cpg	626.37	J/mol×K	1178.61	Joback Method
cpg	630.28	J/mol×K	1226.19	Joback Method
cpg	632.90	J/mol×K	1273.77	Joback Method
cpg	634.24	J/mol×K	1321.36	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C2475458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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