9,10-Anthracenedione, 1,4-bis(methylamino)-

Other names:	Acetate Blue B
	Anthraquinone, 1,4-bis(methylamino)-
	Artisil Blue BRP
	1,4-Bis(methylamino)anthraquinone
	1,4-Bis(methylamino)-9,10-anthraquinone
	Celliton Fast Blue B
	Cibacet Blue BR
	Cilla Fast Blue B
	C.I. 61500
	C.I. Disperse Blue 14
	C.I. Disperse Blue 78
	C.I. Disperse Blue 110
	Disperse Blue 14
	Duranol Brilliant Blue G
	Resiren Blue TB
	Serisol Brilliant Blue G
	Setacyl Blue BS
	Supracet Fast Blue 2G
	Disperse Blue 78
	Solvent Blue 78
	Teraprint Blue R
	1,4-Bis(methylamino)-9,10-anthracenedione
	1,4-Bis(N-methylamino)anthraquinone
	C.I. Solvent Blue 78
	C.I. Solvent Blue 93
	Diaresin Blue K
	Disperse Blue 110
	Macrolex Blue FR
	NSC 86161
	Solvent Blue 93
	1,4-bis(N-methylamino)anthra-9,10-quinone
Inchi:	InChI=1S/C16H14N2O2/c1-17-11-7-8-12(18-2)14-13(11)15(19)9-5-3-4-6-10(9)16(14)20/h
InchiKey:	QOSTVEDABRQTSU-UHFFFAOYSA-N
Formula:	C16H14N2O2
SMILES:	CNc1ccc(NC)c2c1C(=O)c1ccccc1C2=O
Mol. weight [g/mol]:	266.29
CAS:	2475-44-7

Physical Properties

Property code	Value	Unit	Source
gf	284.30	kJ/mol	Joback Method
hf	-15.55	kJ/mol	Joback Method
hfus	32.10	kJ/mol	Joback Method
hvap	79.83	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.545		Crippen Method
mcvol	201.020	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	881.88	K	Joback Method
tc	1137.33	K	Joback Method
tf	640.46	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.42	J/mol×K	881.88	Joback Method
cpg	619.22	J/mol×K	924.46	Joback Method
cpg	630.78	J/mol×K	967.03	Joback Method
cpg	641.14	J/mol×K	1009.61	Joback Method
cpg	650.34	J/mol×K	1052.18	Joback Method
cpg	658.42	J/mol×K	1094.76	Joback Method
cpg	665.41	J/mol×K	1137.33	Joback Method
hsubt	151.80 ± 3.90	kJ/mol	399.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2475447&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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