9,10-Anthracenedione, 1,4-diamino-5-nitro-

Other names:	Anthraquinone, 1,4-diamino-5-nitro-
	C.I. Disperse Violet 8
	C.I. 62030
	Celliton Fast Violet B
	Celliton Fast Violet BA-CF
	Celliton Violet B
	Cibacet Brilliant Violet 3B
	Cilla Fast Violet B
	Diacelliton Fast Violet B
	Dianix Fast Violet B
	Disperse Violet 2S
	Duranol Brilliant Blue Violet BR
	Duranol Brilliant Violet BR
	Fenacet Fast Violet B
	Kayalon Fast Violet BR
	Miketon Fast Violet B
	Nitrocresolamine
	Palanil Violet 3B
	Perliton Violet B
	Samaron Brilliant Violet B
	Serisol Fast Violet B
	Supracet Fast Violet B
	Terasil Brilliant Violet 3B
	Vonteryl Violet 2B
	1,4-Diamino-5-nitroanthraquinone
	5-Nitro-1,4-diaminoanthraquinone
	Disperse Violet 8
	Violet 2S
	NSC 81260
Inchi:	InChI=1S/C14H9N3O4/c15-7-4-5-8(16)12-11(7)13(18)6-2-1-3-9(17(20)21)10(6)14(12)19/
InchiKey:	SDICTISQCKLMEB-UHFFFAOYSA-N
Formula:	C14H9N3O4
SMILES:	Nc1ccc(N)c2c1C(=O)c1cccc([N+](=O)[O-])c1C2=O
Mol. weight [g/mol]:	283.24
CAS:	82-33-7

Physical Properties

Property code	Value	Unit	Source
gf	247.50	kJ/mol	Joback Method
hf	-35.86	kJ/mol	Joback Method
hfus	38.09	kJ/mol	Joback Method
hvap	101.04	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	1.535		Crippen Method
mcvol	190.260	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
tb	1037.66	K	Joback Method
tc	1330.63	K	Joback Method
tf	835.25	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.78	J/mol×K	1037.66	Joback Method
cpg	591.22	J/mol×K	1086.49	Joback Method
cpg	597.31	J/mol×K	1135.32	Joback Method
cpg	602.08	J/mol×K	1184.14	Joback Method
cpg	605.58	J/mol×K	1232.97	Joback Method
cpg	607.83	J/mol×K	1281.80	Joback Method
cpg	608.87	J/mol×K	1330.63	Joback Method

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=C82337&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
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