Isoviolanthrone

Other names:	Benzo[rst]phenanthro[10,1,2-cde]pentaphene-9,18-dione
	Benzadone Violet B
	C.I. Vat Violet 10
	C.I. 60000
	Carbanthrene Printing Violet 2R
	Dinaphtho(1,2,3-cd:1',2',3'-lm)perylene-9,18-dione
	Isodibenzanthrone
	Isothrene
	Isoviolanthrone A
	Izodibenzantron
	Paradone Brilliant Violet 2R
	Paradone Violet B New
	Romantrene Brilliant Violet F2R
	Romantrene Brilliant Violet F4R
	Romantrene Brilliant Violet 4R
	Romantrene Violet 2R
	NSC 5268
	Isodibenzanthrone (isoviolanthrone)
Inchi:	InChI=1S/C34H16O2/c35-33-25-7-3-1-5-17(25)19-9-11-21-24-14-16-28-32-20(18-6-2-4-8
InchiKey:	BSIHWSXXPBAGTC-UHFFFAOYSA-N
Formula:	C34H16O2
SMILES:	O=C1c2ccccc2-c2ccc3c4ccc5c6c(ccc(c7ccc1c2c73)c64)-c1ccccc1C5=O
Mol. weight [g/mol]:	456.49
CAS:	128-64-3

Physical Properties

Property code	Value	Unit	Source
gf	846.94	kJ/mol	Joback Method
hf	515.61	kJ/mol	Joback Method
hfus	55.04	kJ/mol	Joback Method
hvap	118.24	kJ/mol	Joback Method
log10ws	-13.72		Crippen Method
logp	8.160		Crippen Method
mcvol	326.520	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
tb	1311.78	K	Joback Method
tc	1614.52	K	Joback Method

tf	996.84	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1171.86	J/mol×K	1311.78	Joback Method
cpg	1212.38	J/mol×K	1362.24	Joback Method
cpg	1257.73	J/mol×K	1412.69	Joback Method
cpg	1308.49	J/mol×K	1463.15	Joback Method
cpg	1365.28	J/mol×K	1513.61	Joback Method
cpg	1428.68	J/mol×K	1564.06	Joback Method
cpg	1499.29	J/mol×K	1614.52	Joback Method
hsubt	221.10	kJ/mol	538.00	NIST Webbook
hsubt	215.50	kJ/mol	537.00	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=C128643&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

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