C.I. Vat Blue 6

Other names:	VAT Blue 6
	C.I. Vat Blue 6
Inchi:	InChI=1S/C28H12Cl2N2O4/c29-17-9-15-19(27(35)13-7-3-1-5-11(13)25(15)33)23-21(17)3
InchiKey:	UGCDBQWJXSAYIL-UHFFFAOYSA-N
Formula:	C28H12Cl2N2O4
SMILES:	O=c1c2ccccc2c(=O)c2c1cc(Cl)c1[nH]c3c([nH]c12)c(Cl)cc1c(=O)c2ccccc2c(=O)c13
Mol. weight [g/mol]:	511.32

Physical Properties

Property code	Value	Unit	Source
hf	-12.83	kJ/mol	Cheméo Relay (1.0)
ie	7.76	eV	Cheméo Relay (1.0)
logp	4.484		Crippen Method
mcvol	328.480	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	199.00	kJ/mol	576.50	NIST Webbook

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C130201&Units=SI
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):	

Legend

hf:	Enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume