

7,16-dichloro-6,15-dihydroanthrazine-5,9,14,18-tetraone

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)
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]:	511.31
CAS:	130-20-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.21		Crippen Method
logp	4.484		Crippen Method
mvol	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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C130201&Units=SI

Legend

hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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