5,7-dibromo-2-(5,7-dibromo-1,3-dihydro-3-oxo-2H-

Other names: 5,7-Dibromo-2-(5,7-dibromo-1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one (C.I. Vat Blue 5)

Inchi: InChI=1S/C16H6Br4N2O2/c17-5-1-7-11(9(19)3-5)21-13(15(7)23)14-16(24)8-2-6(18)4-10

InchiKey: PTWYQANXSNMUTI-BUHFOSPRSA-N

Formula: C16H6Br4N2O2

SMILES: O=C1C(=C2Nc3c(Br)cc(Br)cc3C2=O)Nc2c(Br)cc(Br)cc21

Mol. weight [g/mol]: 577.85

CAS: 2475-31-2

Physical Properties

Property code	Value	Unit	Source
gf	386.02	kJ/mol	Joback Method
hf	157.33	kJ/mol	Joback Method
hfus	56.86	kJ/mol	Joback Method
hvap	109.54	kJ/mol	Joback Method
log10ws	-8.91		Crippen Method
logp	5.865		Crippen Method
mcvol	255.860	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
tb	1178.04	K	Joback Method
tc	1495.61	K	Joback Method
tf	1053.90	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.90	J/mol×K	1442.68	Joback Method
cpg	627.14	J/mol×K	1178.04	Joback Method
cpg	635.06	J/mol×K	1230.97	Joback Method
cpg	642.47	J/mol×K	1283.90	Joback Method
cpg	649.51	J/mol×K	1336.82	Joback Method
cpg	656.27	J/mol×K	1389.75	Joback Method
cpg	669.50	J/mol×K	1495.61	Joback Method
hsubt	129.00	kJ/mol	576.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2475312&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