6-chloro-2-(6-chloro-4-methyl-3-oxobenzo[b]thien

Other names: 6-Chloro-2-(6-chloro-4-methyl-3-oxobenzo[b]thien-2(3H)-ylidine)-4-methyl-benzo[b]thioph (C.I. Vat Red 1)

Inchi: InChI=1S/C18H10Cl2O2S2/c1-7-3-9(19)5-11-13(7)15(21)17(23-11)18-16(22)14-8(2)4-10

InchiKey: NDDLLTAIKYHPOD-ISLYRVAYSA-N

Formula: C18H10Cl2O2S2

SMILES: Cc1cc(Cl)cc2c1C(=O)C(=C1Sc3cc(Cl)cc(C)c3C1=O)S2

Mol. weight [g/mol]: 393.31

CAS: 2379-74-0

Physical Properties

Property code	Value	Unit	Source
gf	226.02	kJ/mol	Joback Method
hf	-5.85	kJ/mol	Joback Method
hfus	37.42	kJ/mol	Joback Method
hvap	95.13	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	6.099		Crippen Method
mcvol	251.260	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
tb	1032.58	K	Joback Method
tc	1327.16	K	Joback Method
tf	853.92	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.44	J/mol×K	1278.06	Joback Method
cpg	676.32	J/mol×K	1032.58	Joback Method
cpg	686.59	J/mol×K	1081.68	Joback Method
cpg	695.84	J/mol×K	1130.77	Joback Method
cpg	704.18	J/mol×K	1179.87	Joback Method
cpg	711.68	J/mol×K	1228.97	Joback Method
cpg	724.55	J/mol×K	1327.16	Joback Method
hsubt	148.00	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
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=C2379740&Units=SI

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