5-chloro-2-(5-chloro-7-methyl-3-oxobenzo[b]thien

Other names: 5-Chloro-2-(5-chloro-7-methyl-3-oxobenzo[b]thien-2(3H)-ylidine)-7-methyl-benzo[b]thioph
Inchi: InChI=1S/C18H10Cl2O2S2/c1-7-3-9(19)5-11-13(21)17(23-15(7)11)18-14(22)12-6-10(20)
(C.I. Vat Violet 2)
InchiKey: HUGACAUYNJDGTB-ISLYRVAYSA-N
Formula: C18H10Cl2O2S2
SMILES: Cc1cc(Cl)cc2c1SC(=C1Sc3c(C)cc(Cl)cc3C1=O)C2=O
Mol. weight [g/mol]: 393.31
CAS: 5462-29-3

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	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	718.44	J/mol×K	1278.06	Joback Method
cpg	724.55	J/mol×K	1327.16	Joback Method
hsubt	93.00	kJ/mol	576.50	NIST Webbook

Sources

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=C5462293&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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