6-(Dimethylaminomethyl)-2,2'-thio-bis-(4-chloroph

Inchi: InChI=1S/C15H15Cl2NO2S/c1-18(2)8-9-5-11(17)7-14(15(9)20)21-13-6-10(16)3-4-12(13)

InchiKey: BKCCKHRWPLAHPA-UHFFFAOYSA-N

Formula: C15H15Cl2NO2S

SMILES: CN(C)Cc1cc(Cl)cc(Sc2cc(Cl)ccc2O)c1O

Mol. weight [g/mol]: 344.26

CAS: 116435-08-6

Physical Properties

Property code	Value	Unit	Source
gf	82.15	kJ/mol	Joback Method
hf	-190.98	kJ/mol	Joback Method
hfus	48.63	kJ/mol	Joback Method
hvap	99.18	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.617		Crippen Method
mcvol	237.240	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
tb	928.22	K	Joback Method
tc	1192.79	K	Joback Method
tf	699.36	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.39	J/mol×K	928.22	Joback Method
cpg	665.07	J/mol×K	972.31	Joback Method
cpg	677.75	J/mol×K	1016.41	Joback Method
cpg	690.64	J/mol×K	1060.50	Joback Method
cpg	703.97	J/mol×K	1104.60	Joback Method
cpg	717.97	J/mol×K	1148.69	Joback Method
cpg	732.85	J/mol×K	1192.79	Joback Method

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=C116435086&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
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