4-Chloro-1-[(4-chloro-2-nitrophenyl)disulfanyl]-2-n

Other names: bis(4-chloro-2-nitrophenyl) disulphide
Inchi: InChI=1S/C12H6Cl2N2O4S2/c13-7-1-3-11(9(5-7)15(17)18)21-22-12-4-2-8(14)6-10(12)16
InchiKey: DESADCWXGJLRSR-UHFFFAOYSA-N
Formula: C12H6Cl2N2O4S2
SMILES: O=[N+]([O-])c1cc(Cl)ccc1SSc1ccc(Cl)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 377.22
CAS: 2050-66-0

Physical Properties

Property code	Value	Unit	Source
gf	349.94	kJ/mol	Joback Method
hf	166.91	kJ/mol	Joback Method
hfus	52.74	kJ/mol	Joback Method
hvap	105.09	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	5.609		Crippen Method
mcvol	224.440	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
tb	1063.34	K	Joback Method
tc	1380.15	K	Joback Method
tf	743.78	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.15	J/mol×K	1063.34	Joback Method
cpg	562.14	J/mol×K	1116.14	Joback Method
cpg	564.71	J/mol×K	1168.94	Joback Method
cpg	565.93	J/mol×K	1221.75	Joback Method
cpg	565.89	J/mol×K	1274.55	Joback Method
cpg	564.66	J/mol×K	1327.35	Joback Method
cpg	562.30	J/mol×K	1380.15	Joback Method

Sources

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=C2050660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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