4-Chloro-4'-nitrodiphenyl sulfide

Other names:	4-Nitro-4'-chloro diphenyl sulfide
	Benzene, 1-chloro-4-[(4-nitrophenyl)thio]-
Inchi:	InChI=1S/C12H8ClNO2S/c13-9-1-5-11(6-2-9)17-12-7-3-10(4-8-12)14(15)16/h1-8H
InchiKey:	CPUBRDUBQIVBGM-UHFFFAOYSA-N
Formula:	C12H8ClNO2S
SMILES:	O=[N+]([O-])c1ccc(Sc2ccc(Cl)cc2)cc1
Mol. weight [g/mol]:	265.71
CAS:	21969-11-9

Physical Properties

Property code	Value	Unit	Source
gf	312.46	kJ/mol	Joback Method
hf	174.48	kJ/mol	Joback Method
hfus	33.83	kJ/mol	Joback Method
hvap	75.97	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.399		Crippen Method
mcvol	178.430	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	795.33	K	Joback Method
tc	1088.59	K	Joback Method
tf	510.81	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.08	J/mol×K	795.33	Joback Method
cpg	449.23	J/mol×K	844.21	Joback Method
cpg	459.05	J/mol×K	893.08	Joback Method
cpg	467.64	J/mol×K	941.96	Joback Method
cpg	475.10	J/mol×K	990.84	Joback Method
cpg	481.52	J/mol×K	1039.71	Joback Method
cpg	486.99	J/mol×K	1088.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21969119&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
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