

4,4'-Diaminodiphenyl disulphide

Other names:	4-Aminophenyldisulfide p-p'-Dithiodianiline 4,4'-Diaminodiphenyl disulfide Benzenamine, 4,4'-dithiobis- Aniline, p,p'-dithiodi- 4,4'-Dithiodianiline
Inchi:	InChI=1S/C12H12N2S2/c13-9-1-5-11(6-2-9)15-16-12-7-3-10(14)4-8-12/h1-8H,13-14H2
InchiKey:	MERLDGDYUMSLAY-UHFFFAOYSA-N
Formula:	C12H12N2S2
SMILES:	<chem>Nc1ccc(SSc2ccc(N)cc2)cc1</chem>
Mol. weight [g/mol]:	248.37
CAS:	722-27-0

Physical Properties

Property code	Value	Unit	Source
gf	454.86	kJ/mol	Joback Method
hf	310.43	kJ/mol	Joback Method
hfus	32.79	kJ/mol	Joback Method
hvap	83.10	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.650		Crippen Method
mcvol	185.080	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
tb	819.90	K	Joback Method
tc	1116.63	K	Joback Method
tf	538.20	K	Joback Method
vc	0.657	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.05	J/mol×K	819.90	Joback Method
cpg	495.95	J/mol×K	869.35	Joback Method
cpg	506.36	J/mol×K	918.81	Joback Method

cpg	515.35	J/mol×K	968.26	Joback Method
cpg	523.00	J/mol×K	1017.72	Joback Method
cpg	529.38	J/mol×K	1067.17	Joback Method
cpg	534.57	J/mol×K	1116.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C722270&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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