

Disulfide, bis(4-methylphenyl)

Other names:	p-Tolyl disulfide Biodylon Bis(p-tolyl) disulfide Bis(4-methylphenyl) disulfide Bis(4-tolyl) disulfide Di-p-Tolyl disulfide Di-4-tolyl disulfide Kresulfin 4-Methylphenyl disulfide Di(4-methylphenyl) disulfide 4-Tolyl disulfide Bis(p-methylphenyl) disulfide NSC 677466 NSC 994 di-p-tolyl disulphide
Inchi:	InChI=1S/C14H14S2/c1-11-3-7-13(8-4-11)15-16-14-9-5-12(2)6-10-14/h3-10H,1-2H3
InchiKey:	TZOVOLUMXXLOJ-UHFFFAOYSA-N
Formula:	C14H14S2
SMILES:	<chem>Cc1ccc(SSc2ccc(C)cc2)cc1</chem>
Mol. weight [g/mol]:	246.39
CAS:	103-19-5

Physical Properties

Property code	Value	Unit	Source
gf	338.80	kJ/mol	Joback Method
hf	201.57	kJ/mol	Joback Method
hfus	27.58	kJ/mol	Joback Method
hvap	66.27	kJ/mol	Joback Method
ie	7.50	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-5.71		Crippen Method
logp	5.103		Crippen Method
mcvol	193.300	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
tb	720.60	K	Joback Method
tc	997.89	K	Joback Method
tf	394.22	K	Joback Method

vc

0.712

m³/kmol

Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.57	J/mol×K	720.60	Joback Method
cpg	493.41	J/mol×K	766.81	Joback Method
cpg	507.76	J/mol×K	813.03	Joback Method
cpg	520.65	J/mol×K	859.24	Joback Method
cpg	532.16	J/mol×K	905.46	Joback Method
cpg	542.35	J/mol×K	951.67	Joback Method
cpg	551.27	J/mol×K	997.89	Joback Method

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=C103195&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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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