p-Tolyl sulfide

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:	TZOVOULUMXXLOJ-UHFFFAOYSA-N
Formula:	C14H14S2
SMILES:	Cc1ccc(SSc2ccc(C)cc2)cc1
Mol. weight [g/mol]:	246.40

Physical Properties

Property code	Value	Unit	Source
af	0.4331		Cheméo Relay (1.0)
gf	338.80	kJ/mol	Joback Method
hf	165.43	kJ/mol	Cheméo Relay (1.0)
hfus	27.58	kJ/mol	Joback Method
hvap	89.33	kJ/mol	Cheméo Relay (1.0)
ie	7.50	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-6.21		Cheméo Relay (1.0)
logp	5.103		Crippen Method
mcvol	193.300	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
tb	621.74	K	Cheméo Relay (1.0)
tc	840.49	K	Cheméo Relay (1.0)
tf	361.66	K	Cheméo Relay (1.0)

vc	0.695	m3/kmol	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103195&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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