1,2-Di(phenylthio) ethane

Other names:	Bis(phenylthio)ethane
	Benzene, 1,1'-[1,2-ethanediylbis(thio)]bis-
	Ethane, 1,2-bis(phenylthio)-
	1,2-Di(phenylthio) ethane
	1,1'-[ethane-1,2-diylbis(thio)]bisbenzene
Inchi:	InChI=1S/C14H14S2/c1-3-7-13(8-4-1)15-11-12-16-14-9-5-2-6-10-14/h1-10H,11-12H2
InchiKey:	MHCVYAFXPIMYRD-UHFFFAOYSA-N
Formula:	C14H14S2
SMILES:	c1ccc(SCCSc2ccccc2)cc1
Mol. weight [g/mol]:	246.40

Physical Properties

Property code	Value	Unit	Source
af	0.4040		Cheméo Relay (1.0)
hf	233.32	kJ/mol	Cheméo Relay (1.0)
hfus	28.36	kJ/mol	Joback Method
hvap	97.70	kJ/mol	Cheméo Relay (1.0)
ie	8.26	eV	Cheméo Relay (1.0)
log10ws	-5.67		Cheméo Relay (1.0)
logp	4.571		Crippen Method
mcvol	193.300	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
tb	638.44	K	Cheméo Relay (1.0)
tc	847.20	K	Cheméo Relay (1.0)
tf	346.23	K	Cheméo Relay (1.0)
vc	0.683	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.05	J/mol×K	710.64	Joback Method
cpg	496.26	J/mol×K	756.58	Joback Method
cpg	510.88	J/mol×K	802.52	Joback Method
cpg	524.00	J/mol×K	848.46	Joback Method

cpg	535.71	J/mol×K	894.40	Joback Method
cpg	546.09	J/mol×K	940.35	Joback Method
cpg	555.23	J/mol×K	986.29	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C622208&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
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