trans-1,2-Bis(benzylthio)-ethylene

Inchi: InChI=1S/C16H16S2/c1-3-7-15(8-4-1)13-17-11-12-18-14-16-9-5-2-6-10-16/h1-12H,13-14
InchiKey: RZVCNFNSLCXUMM-VAWYXSNFSA-N
Formula: C16H16S2
SMILES: C(=CSCc1ccccc1)SCc1ccccc1
Mol. weight [g/mol]: 272.43
CAS: 788-26-1

Physical Properties

Property code	Value	Unit	Source
chg	-9923.90 ± 1.20	kJ/mol	NIST Webbook
gf	455.12	kJ/mol	Joback Method
hf	300.45	kJ/mol	Joback Method
hfl	136.60	kJ/mol	NIST Webbook
hfus	33.74	kJ/mol	Joback Method
hvap	69.35	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.324		Crippen Method
mcvol	217.180	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
tb	760.56	K	Joback Method
tc	1033.56	K	Joback Method
tf	386.64	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.22	J/mol×K	760.56	Joback Method
cpg	577.37	J/mol×K	806.06	Joback Method
cpg	591.96	J/mol×K	851.56	Joback Method
cpg	605.13	J/mol×K	897.06	Joback Method
cpg	617.01	J/mol×K	942.56	Joback Method
cpg	627.70	J/mol×K	988.06	Joback Method
cpg	637.35	J/mol×K	1033.56	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=C788261&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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