Benzene, [(phenylmethyl)thio]-

Other names:	Benzyl phenyl sulfide
	Phenyl benzyl sulfide
	Sulfide, benzyl phenyl
	1,2-Diphenyl-1-thiaethane
	benzyl phenyl sulphide
Inchi:	InChI=1S/C13H12S/c1-3-7-12(8-4-1)11-14-13-9-5-2-6-10-13/h1-10H,11H2
InchiKey:	LKMCJXXOBRCATQ-UHFFFAOYSA-N
Formula:	C13H12S
SMILES:	c1ccc(CSc2ccccc2)cc1
Mol. weight [g/mol]:	200.30
CAS:	831-91-4

Physical Properties

Property code	Value	Unit	Source
gf	316.52	kJ/mol	Joback Method
hf	203.28	kJ/mol	Joback Method
hfus	21.64	kJ/mol	Joback Method
hsub	98.40 ± 1.40	kJ/mol	NIST Webbook
hvap	55.90	kJ/mol	Joback Method
ie	7.87 ± 0.02	eV	NIST Webbook
log10ws	-4.33		Crippen Method
logp	3.979		Crippen Method
mcvol	162.860	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
tb	618.98	K	Joback Method
tc	883.68	K	Joback Method
tf	323.51	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.75	J/mol×K	618.98	Joback Method
cpg	394.36	J/mol×K	663.10	Joback Method

cpg	409.52	J/mol×K	707.21	Joback Method
cpg	423.31	J/mol×K	751.33	Joback Method
cpg	435.82	J/mol×K	795.45	Joback Method
cpg	447.13	J/mol×K	839.56	Joback Method
cpg	457.34	J/mol×K	883.68	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	470.20	K	3.60	NIST Webbook

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=C831914&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
hsub: Enthalpy of sublimation 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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume