Benzyl sulfide

Other names:	Benzyl monosulfide
	Benzene, 1,1'-[thiobis(methylene)]bis-
	Benzyl thioether
	Dibenzyl monosulfide
	Dibenzyl sulfide
	1,3-Diphenyl-2-thiapropane
	Sulfide, dibenzyl-
	[(Benzylsulfanyl)methyl]benzene
	((Benzylthio)methyl)benzene
	1,1'-(Thiobis(methylene))bisbenzene
	Dibenzyl thioether
	NSC 212544
	Sulfide, benzyl-
	dibenzyl sulphide
Inchi:	InChI=1S/C14H14S/c1-3-7-13(8-4-1)11-15-12-14-9-5-2-6-10-14/h1-10H,11-12H2
InchiKey:	LUFPJJNWMYZRQE-UHFFFAOYSA-N
Formula:	C14H14S
SMILES:	c1ccc(CSCc2ccccc2)cc1
Mol. weight [g/mol]:	214.33
CAS:	538-74-9

Physical Properties

Property code	Value	Unit	Source
chs	-8211.20 ± 2.00	kJ/mol	NIST Webbook
gf	324.94	kJ/mol	Joback Method
hf	193.00 ± 4.20	kJ/mol	NIST Webbook
hfs	99.30 ± 2.00	kJ/mol	NIST Webbook
hfus	24.23	kJ/mol	Joback Method
hsub	94.00 ± 2.00	kJ/mol	NIST Webbook
hsub	93.70	kJ/mol	NIST Webbook
hvap	58.13	kJ/mol	Joback Method
ie	8.05 ± 0.02	eV	NIST Webbook
ie	8.05	eV	NIST Webbook
ie	8.28	eV	NIST Webbook
log10ws	-4.76		Crippen Method
logp	4.120		Crippen Method
mcvol	176.950	ml/mol	McGowan Method

pc	2820.33	kPa	Joback Method
rinpol	2146.80		NIST Webbook
rinpol	2145.90		NIST Webbook
rinpol	2146.80		NIST Webbook
rinpol	2145.90		NIST Webbook
tb	641.86	K	Joback Method
tc	900.23	K	Joback Method
tf	320.00 ± 3.00	K	NIST Webbook
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.35	J/mol×K	641.86	Joback Method
cpg	444.50	J/mol×K	684.92	Joback Method
cpg	460.19	J/mol×K	727.98	Joback Method
cpg	474.51	J/mol×K	771.05	Joback Method
cpg	487.54	J/mol×K	814.11	Joback Method
cpg	499.38	J/mol×K	857.17	Joback Method
cpg	510.10	J/mol×K	900.23	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=C538749&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions

hfs:	Solid phase 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume