Benzyl methyl sulfide

Other names:	Benzene, [(methylthio)methyl]-
	Sulfide, benzyl methyl
	Methyl benzyl sulfide
	1-Phenyl-2-thiapropane
	Methylthiomethylbenzene
	«alpha»-(Methylthio)toluene
	Benzyl methyl sulphide
	NSC 75125
Inchi:	InChI=1S/C8H10S/c1-9-7-8-5-3-2-4-6-8/h2-6H,7H2,1H3
InchiKey:	OFQPKKGMNWASPN-UHFFFAOYSA-N
Formula:	C8H10S
SMILES:	CSCc1ccccc1
Mol. weight [g/mol]:	138.23
CAS:	766-92-7

Physical Properties

Property code	Value	Unit	Source
chl	-5205.10 ± 2.00	kJ/mol	NIST Webbook
gf	162.01	kJ/mol	Joback Method
hf	79.00 ± 3.00	kJ/mol	NIST Webbook
hfl	26.00 ± 2.00	kJ/mol	NIST Webbook
hfus	14.65	kJ/mol	Joback Method
hvap	54.00 ± 2.00	kJ/mol	NIST Webbook
hvap	53.00	kJ/mol	NIST Webbook
hvap	55.20 ± 2.10	kJ/mol	NIST Webbook
ie	8.42	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.64	eV	NIST Webbook
ie	8.41	eV	NIST Webbook
log10ws	-2.65		Crippen Method
logp	2.550		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
rinpol	1176.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1147.00		NIST Webbook

rinpol	1184.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1183.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1665.00		NIST Webbook
ripol	1665.00		NIST Webbook
tb	469.70	K	NIST Webbook
tc	712.59	K	Joback Method
tf	240.74	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.99	J/mol×K	477.90	Joback Method
cpg	236.28	J/mol×K	517.01	Joback Method
cpg	248.73	J/mol×K	556.13	Joback Method
cpg	260.36	J/mol×K	595.24	Joback Method
cpg	271.21	J/mol×K	634.36	Joback Method
cpg	281.31	J/mol×K	673.47	Joback Method
cpg	290.68	J/mol×K	712.59	Joback Method
hvapt	51.80	kJ/mol	352.00	NIST Webbook
hvapt	50.80	kJ/mol	352.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C766927&Units=SI

Legend

chl:	Standard liquid 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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume