Benzene, [(methylsulfinyl)methyl]-

Other names:	Sulfoxide, benzyl methyl
	Benzyl methyl sulfoxide
	DS 1
	Methyl benzyl sulfoxide
	«alpha»-(methylsulphinyl)toluene
Inchi:	InChI=1S/C8H10OS/c1-10(9)7-8-5-3-2-4-6-8/h2-6H,7H2,1H3
InchiKey:	LISVNGUOWUKZQY-UHFFFAOYSA-N
Formula:	C8H10OS
SMILES:	CS(=O)Cc1ccccc1
Mol. weight [g/mol]:	154.23
CAS:	824-86-2

Physical Properties

Property code	Value	Unit	Source
gf	-88.82	kJ/mol	Joback Method
hf	-177.66	kJ/mol	Joback Method
hfus	18.27	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.565		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
tb	467.40	K	Joback Method
tc	685.96	K	Joback Method
tf	242.82	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.21	J/mol×K	467.40	Joback Method
cpg	249.54	J/mol×K	503.83	Joback Method
cpg	262.08	J/mol×K	540.25	Joback Method
cpg	273.87	J/mol×K	576.68	Joback Method

cpg	284.92	J/mol×K	613.11	Joback Method
cpg	295.25	J/mol×K	649.53	Joback Method
cpg	304.87	J/mol×K	685.96	Joback Method

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=C824862&Units=SI

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
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