Benzene, [(methylsulfonyl)methyl]-

Other names:	Benzyl methyl sulfone
	Methyl benzyl sulfone
	Sulfone, benzyl methyl
	«alpha»-(methylsulphonyl)toluene
	Â«alphaÂ»-(methylsulphonyl)toluene
Inchi:	InChI=1S/C8H10O2S/c1-11(9,10)7-8-5-3-2-4-6-8/h2-6H,7H2,1H3
InchiKey:	BEARMXYKACECDH-UHFFFAOYSA-N
Formula:	C8H10O2S
SMILES:	CS(=O)(=O)Cc1ccccc1
Mol. weight [g/mol]:	170.23
CAS:	3112-90-1

Physical Properties

Property code	Value	Unit	Source
chs	-4808.30 ± 3.00	kJ/mol	NIST Webbook
gf	-339.65	kJ/mol	Joback Method
hf	-285.00 ± 4.20	kJ/mol	NIST Webbook
hf	-272.00 ± 4.00	kJ/mol	NIST Webbook
hfs	-374.00 ± 1.00	kJ/mol	NIST Webbook
hfs	-371.00 ± 2.00	kJ/mol	NIST Webbook
hfus	21.89	kJ/mol	Joback Method
hsub	99.00 ± 3.00	kJ/mol	NIST Webbook
hvap	54.31	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.231		Crippen Method
mcvol	127.910	ml/mol	McGowan Method
pc	4444.44	kPa	Joback Method
tb	456.90	K	Joback Method
tc	660.54	K	Joback Method
tf	400.50 ± 0.50	K	NIST Webbook
tf	400.50 ± 0.60	K	NIST Webbook
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.95	J/mol×K	456.90	Joback Method
cpg	262.27	J/mol×K	490.84	Joback Method
cpg	274.88	J/mol×K	524.78	Joback Method
cpg	286.79	J/mol×K	558.72	Joback Method
cpg	298.00	J/mol×K	592.66	Joback Method
cpg	308.54	J/mol×K	626.60	Joback Method
cpg	318.41	J/mol×K	660.54	Joback Method
hfust	25.52	kJ/mol	400.50	NIST Webbook
hfust	25.52	kJ/mol	400.50	NIST Webbook
hvapt	64.90	kJ/mol	492.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.74651e+01
Coeff. B	-7.81037e+03
Temperature range (K), min.	454.69
Temperature range (K), max.	642.64

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=C3112901&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume