

BENZENE, (METHYLSULFONYL)-

Other names:	Benzene, (methylsulfonyl)- Methyl phenyl sulfone Phenyl methyl sulfone (Methylsulphonyl)benzene Methyl phenyl sulphone (Phenylsulfonyl)methane (Methylsulfonyl)benzene NSC 41587
Inchi:	InChI=1S/C7H8O2S/c1-10(8,9)7-5-3-2-4-6-7/h2-6H,1H3
InchiKey:	JCDWETOKTFWTHA-UHFFFAOYSA-N
Formula:	C7H8O2S
SMILES:	CS(=O)(=O)c1ccccc1
Mol. weight [g/mol]:	156.21

Physical Properties

Property code	Value	Unit	Source
affp	812.70	kJ/mol	NIST Webbook
basg	780.30	kJ/mol	NIST Webbook
chl	-4154.80 ± 0.67	kJ/mol	NIST Webbook
hf	-253.40 ± 3.10	kJ/mol	NIST Webbook
hfl	-345.40 ± 0.88	kJ/mol	NIST Webbook
hfus	19.30	kJ/mol	Joback Method
hvap	85.00	kJ/mol	Cheméo Relay (1.0)
ie	9.74	eV	NIST Webbook
ie	9.85	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
log10ws	-1.97		Cheméo Relay (1.0)
logp	1.090		Crippen Method
mcvol	113.820	ml/mol	McGowan Method
tb	560.34	K	Cheméo Relay (1.0)
tf	361.00 ± 3.00	K	NIST Webbook
tf	359.00 ± 3.00	K	NIST Webbook
tf	360.00 ± 3.00	K	NIST Webbook
tf	363.00 ± 2.00	K	NIST Webbook
tf	358.00 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.52	J/mol×K	434.02	Joback Method
cpg	220.66	J/mol×K	468.38	Joback Method
cpg	232.16	J/mol×K	502.74	Joback Method
cpg	243.01	J/mol×K	537.10	Joback Method
cpg	253.24	J/mol×K	571.45	Joback Method
cpg	262.84	J/mol×K	605.81	Joback Method
cpg	271.83	J/mol×K	640.17	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3112854&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

tf: Normal melting (fusion) point

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