

Benzenemethanesulfonyl chloride

Other names:	«alpha»-Toluenesulfonyl chloride Benzylsulfochloride Benzylsulfonyl chloride Methanesulfonyl chloride, phenyl- Phenylmethanesulfonyl chloride Phenylmethane sulfo chloride Phenylmethylsulfonyl chloride toluene-«alpha»-sulphonyl chloride
Inchi:	InChI=1S/C7H7ClO2S/c8-11(9,10)6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	OAHKWDDSKCRNFE-UHFFFAOYSA-N
Formula:	C7H7ClO2S
SMILES:	O=S(=O)(Cl)Cc1ccccc1
Mol. weight [g/mol]:	190.65
CAS:	1939-99-7

Physical Properties

Property code	Value	Unit	Source
gf	-360.00	kJ/mol	Joback Method
hf	-420.37	kJ/mol	Joback Method
hfus	23.50	kJ/mol	Joback Method
hvap	56.47	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	1.755		Crippen Method
mcvol	126.060	ml/mol	McGowan Method
pc	4815.84	kPa	Joback Method
tb	471.45	K	Joback Method
tc	684.11	K	Joback Method
tf	263.55	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.21	J/mol×K	471.45	Joback Method

cpg	245.76	J/mol×K	506.89	Joback Method
cpg	256.62	J/mol×K	542.34	Joback Method
cpg	266.79	J/mol×K	577.78	Joback Method
cpg	276.28	J/mol×K	613.22	Joback Method
cpg	285.12	J/mol×K	648.67	Joback Method
cpg	293.31	J/mol×K	684.11	Joback Method

Sources

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=C1939997&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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