

Benzenesulfonyl chloride

Other names:	Benzene sulfochloride
	Benzene sulfonechloride
	Benzenesulfonic chloride
	Phenylsulfonyl chloride
	Benzenesulfonic acid chloride
	Benzenosulfochlorek
	Benzenosulfochloride
	Benzene sulphonyl chloride
	NSC 2864
Inchi:	InChI=1S/C6H5ClO2S/c7-10(8,9)6-4-2-1-3-5-6/h1-5H
InchiKey:	CSKNSYBAZOQPLR-UHFFFAOYSA-N
Formula:	C6H5ClO2S
SMILES:	O=S(=O)(Cl)c1ccccc1
Mol. weight [g/mol]:	176.62
CAS:	98-09-9

Physical Properties

Property code	Value	Unit	Source
gf	-368.42	kJ/mol	Joback Method
hf	-399.73	kJ/mol	Joback Method
hfus	20.91	kJ/mol	Joback Method
hvap	54.25	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.614		Crippen Method
mcvol	111.970	ml/mol	McGowan Method
pc	5527.84	kPa	Joback Method
tb	448.57	K	Joback Method
tc	664.27	K	Joback Method
tf	252.28	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
---------------	-------	------	-----------------	--------

cpg	194.55	J/mol×K	448.57	Joback Method
cpg	204.85	J/mol×K	484.52	Joback Method
cpg	214.53	J/mol×K	520.47	Joback Method
cpg	223.58	J/mol×K	556.42	Joback Method
cpg	232.03	J/mol×K	592.37	Joback Method
cpg	239.87	J/mol×K	628.32	Joback Method
cpg	247.12	J/mol×K	664.27	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=C98099&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

Latest version available from:

<https://www.chemeo.com/cid/98-605-2/Benzenesulfonyl-chloride.pdf>

Generated by Cheméo on 2025-12-05 23:31:52.070238609 +0000 UTC m=+4725709.600279272.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.