Benzenesulfonamide

Other names:	BSA
	Benzenesulphonamide
	Benzosulfonamide
Inchi:	InChI=1S/C6H7NO2S/c7-10(8,9)6-4-2-1-3-5-6/h1-5H,(H2,7,8,9)
InchiKey:	KHBQMWCZKVMBLN-UHFFFAOYSA-N
Formula:	C6H7NO2S
SMILES:	NS(=O)(=O)c1ccccc1
Mol. weight [g/mol]:	157.19
CAS:	98-10-2

Physical Properties

Property code	Value	Unit	Source
chs	-3400.00	kJ/mol	NIST Webbook
gf	-290.04	kJ/mol	Joback Method
hf	-350.20	kJ/mol	Joback Method
hfs	-561.90	kJ/mol	NIST Webbook
hfus	23.74	kJ/mol	Enthalpies of combustion and formation of benzenesulfonamide and some of its derivatives
hsub	115.30 ± 1.70	kJ/mol	NIST Webbook
hvap	60.50	kJ/mol	Joback Method
log10ws	-1.56		Aqueous Solubility Prediction Method
logp	0.334		Crippen Method
mcvol	109.710	ml/mol	McGowan Method
pc	6389.77	kPa	Joback Method
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
tb	483.67	K	Joback Method
tc	705.60	K	Joback Method
tf	424.82	K	Aqueous Solubility Prediction Method
tf	429.65 ± 1.00	K	NIST Webbook
tf	425.35	K	Solubility Determination, Modeling, and Thermodynamic Dissolution Properties of Benzenesulfonamide in 16 Neat Solvents from 273.15 to 324.45 K

vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.71	J/mol×K	483.67	Joback Method
cpg	230.91	J/mol×K	520.66	Joback Method
cpg	241.40	J/mol×K	557.65	Joback Method
cpg	251.19	J/mol×K	594.64	Joback Method
cpg	260.29	J/mol×K	631.62	Joback Method
cpg	268.72	J/mol×K	668.61	Joback Method
cpg	276.47	J/mol×K	705.60	Joback Method
cps	193.30	J/mol×K	323.00	NIST Webbook
hfust	25.17	kJ/mol	425.80	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98102&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Enthalpies of combustion and formation of benzenesulfonamide and some of its derivatives:	https://www.doi.org/10.1016/j.jct.2011.11.026
Solubilities of benzenesulfonamide in supercritical CO2 in the absence and presence of cosolvent:	https://www.doi.org/10.1016/j.tca.2011.10.023
Solubility Determination, Modeling, and Thermodynamic Dissolution Properties of Benzenesulfonamide in 16 Neat Solvents from 273.15 to 324.45 K:	https://www.doi.org/10.1021/acs.jced.9b00360
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume