(Phenylsulfonyl)acetonitrile

Other names:	Acetonitrile, (phenylsulfonyl)-
	Acetonitrile, 2-phenylsulfonyl-
	Benzenesulfonyl-acetonitrile
	Phenylsulphonylacetonitrile
Inchi:	InChI=1S/C8H7NO2S/c9-6-7-12(10,11)8-4-2-1-3-5-8/h1-5H,7H2
InchiKey:	ZFCFFNGBCVAUDE-UHFFFAOYSA-N
Formula:	C8H7NO2S
SMILES:	N#CCS(=O)(=O)c1ccccc1
Mol. weight [g/mol]:	181.21
CAS:	7605-28-9

Physical Properties

Property code	Value	Unit	Source
gf	-206.47	kJ/mol	Joback Method
hf	-260.39	kJ/mol	Joback Method
hfus	23.40	kJ/mol	Joback Method
hvap	64.79	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	0.984		Crippen Method
mcvol	129.290	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
tb	558.98	K	Joback Method
tc	781.18	K	Joback Method
tf	309.89	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.00	J/mol×K	558.98	Joback Method
cpg	286.88	J/mol×K	596.01	Joback Method
cpg	297.00	J/mol×K	633.05	Joback Method
cpg	306.39	J/mol×K	670.08	Joback Method
cpg	315.04	J/mol×K	707.12	Joback Method

cpg	322.98	J/mol×K	744.15	Joback Method
cpg	330.21	J/mol×K	781.18	Joback Method

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=C7605289&Units=SI

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