Benzenesulfonyl isocyanate

Other names: phenylsulphonyl isocyanate
Inchi: InChI=1S/C7H5NO3S/c9-6-8-12(10,11)7-4-2-1-3-5-7/h1-5H
InchiKey: UJYAZVSPFMJCLW-UHFFFAOYSA-N
Formula: C7H5NO3S
SMILES: O=C=NS(=O)(=O)c1ccccc1
Mol. weight [g/mol]: 183.18
CAS: 2845-62-7

Physical Properties

Property code	Value	Unit	Source
hf	-410.04	kJ/mol	Joback Method
hvap	61.62	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	0.711		Crippen Method
mcvol	121.070	ml/mol	McGowan Method
pc	5653.23	kPa	Joback Method
tb	500.69	K	Joback Method
tc	717.05	K	Joback Method

Sources

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=C2845627&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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