Propane, 2-[(1,1-dimethylethyl)sulfonyl]-2-methyl-

Other names: Di-tert-Butyl sulfone
tert-Butyl Sulfone
Di-tert-butyl sulphone
2-((1,1-Dimethylethyl)-sulphonyl)-2-methylpropane

Inchi: InChI=1S/C8H18O2S/c1-7(2,3)11(9,10)8(4,5)6/h1-6H3

InchiKey: SPJQDMKTFSPPLO-UHFFFAOYSA-N

Formula: C8H18O2S

SMILES: CC(C)(C)S(=O)(=O)C(C)(C)C

Mol. weight [g/mol]: 178.29

CAS: 1886-75-5

Physical Properties

Property code	Value	Unit	Source
chs	-5682.50 ± 2.20	kJ/mol	NIST Webbook
gf	-446.38	kJ/mol	Joback Method
hf	-546.30 ± 2.50	kJ/mol	NIST Webbook
hfs	-640.40 ± 2.30	kJ/mol	NIST Webbook
hfus	13.03	kJ/mol	Joback Method
hvap	49.45	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.998		Crippen Method
mcvol	151.670	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	521.00 ± 3.00	K	NIST Webbook
tc	606.70	K	Joback Method
tf	403.00 ± 2.00	K	NIST Webbook
tf	403.00 ± 3.00	K	NIST Webbook
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.21	J/mol×K	423.76	Joback Method
cpg	329.64	J/mol×K	454.25	Joback Method

cpg	345.21	J/mol×K	484.74	Joback Method
cpg	359.95	J/mol×K	515.23	Joback Method
cpg	373.87	J/mol×K	545.72	Joback Method
cpg	387.01	J/mol×K	576.21	Joback Method
cpg	399.40	J/mol×K	606.70	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=C1886755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
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