3-Butenyl p-tolyl sulphone

Inchi: InChI=1S/C11H14O2S/c1-3-4-9-14(12,13)11-7-5-10(2)6-8-11/h3,5-8H,1,4,9H2,2H3
InchiKey: KFKSUCUTIOURTG-UHFFFAOYSA-N
Formula: C11H14O2S
SMILES: C=CCCS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 210.29
CAS: 17482-19-8

Physical Properties

Property code	Value	Unit	Source
chs	-6592.30 ± 1.30	kJ/mol	NIST Webbook
gf	-236.18	kJ/mol	Joback Method
hf	-226.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-339.20 ± 1.30	kJ/mol	NIST Webbook
hfus	28.00	kJ/mol	Joback Method
hsub	113.00 ± 3.00	kJ/mol	NIST Webbook
hvap	60.98	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.345		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
tb	527.20	K	Joback Method
tc	728.09	K	Joback Method
tf	289.47	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.71	J/mol×K	527.20	Joback Method
cpg	378.80	J/mol×K	560.68	Joback Method
cpg	393.05	J/mol×K	594.16	Joback Method
cpg	406.49	J/mol×K	627.65	Joback Method
cpg	419.13	J/mol×K	661.13	Joback Method
cpg	430.99	J/mol×K	694.61	Joback Method

cpg	442.08	J/mol×K	728.09	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=C17482198&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume