

But-1-enyl-p-tolyl sulphone

Inchi:	InChI=1S/C11H14O2S/c1-3-4-9-14(12,13)11-7-5-10(2)6-8-11/h4-9H,3H2,1-2H3/b9-4+
InchiKey:	CGOCKBRDRHIVRU-RUDMXATFSA-N
Formula:	C11H14O2S
SMILES:	CCC=CS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	210.29
CAS:	111895-49-9

Physical Properties

Property code	Value	Unit	Source
chs	-6595.70 ± 0.20	kJ/mol	NIST Webbook
gf	-243.80	kJ/mol	Joback Method
hf	-230.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-335.80 ± 1.10	kJ/mol	NIST Webbook
hfus	29.48	kJ/mol	Joback Method
hvap	61.61	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.692		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
tb	534.68	K	Joback Method
tc	740.42	K	Joback Method
tf	286.15	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.54	J/molxK	534.68	Joback Method
cpg	379.79	J/molxK	568.97	Joback Method
cpg	394.15	J/molxK	603.26	Joback Method
cpg	407.65	J/molxK	637.55	Joback Method
cpg	420.31	J/molxK	671.84	Joback Method
cpg	432.15	J/molxK	706.13	Joback Method
cpg	443.21	J/molxK	740.42	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=C111895499&Units=SI

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

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