4-T-amylbenzenesulphonyl chloride

Inchi: InChI=1S/C11H15ClO2S/c1-2-3-4-5-10-6-8-11(9-7-10)15(12,13)14/h6-9H,2-5H2,1H3
InchiKey: XDWXZRVWJHEWMT-UHFFFAOYSA-N
Formula: C11H15ClO2S
SMILES: CCCCCc1ccc(S(=O)(=O)Cl)cc1
Mol. weight [g/mol]: 246.75
CAS: 73948-18-2

Physical Properties

Property code	Value	Unit	Source
gf	-335.95	kJ/mol	Joback Method
hf	-514.40	kJ/mol	Joback Method
hfus	33.47	kJ/mol	Joback Method
hvap	66.04	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.347		Crippen Method
mcvol	182.420	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
tb	567.95	K	Joback Method
tc	769.39	K	Joback Method
tf	321.15	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.33	J/mol×K	567.95	Joback Method
cpg	427.15	J/mol×K	601.52	Joback Method
cpg	441.13	J/mol×K	635.10	Joback Method
cpg	454.27	J/mol×K	668.67	Joback Method
cpg	466.61	J/mol×K	702.24	Joback Method
cpg	478.14	J/mol×K	735.82	Joback Method
cpg	488.89	J/mol×K	769.39	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=C73948182&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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