Cyclohexyl-p-toluene sulfonate

Other names:	Benzenesulfonic acid, 4-methyl-, cyclohexyl ester
	p-Toluenesulfonic acid, cyclohexyl ester
	Cyclohexyl toluenesulfonate
	Cyclohexyl tosylate
	Toluene-4-sulfonic acid, cyclohexyl ester
	cyclohexyl p-toluenesulphonate
Inchi:	InChI=1S/C13H18O3S/c1-11-7-9-13(10-8-11)17(14,15)16-12-5-3-2-4-6-12/h7-10,12H,2-6
InchiKey:	OHHPZPDQZMUTCA-UHFFFAOYSA-N
Formula:	C13H18O3S
SMILES:	Cc1ccc(S(=O)(=O)OC2CCCCC2)cc1
Mol. weight [g/mol]:	254.34
CAS:	953-91-3

Physical Properties

Property code	Value	Unit	Source
gf	-387.73	kJ/mol	Joback Method
hf	-617.84	kJ/mol	Joback Method
hfus	27.48	kJ/mol	Joback Method
hvap	68.94	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.033		Crippen Method
mcvol	193.370	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
tb	618.25	K	Joback Method
tc	842.13	K	Joback Method
tf	343.38	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.58	J/mol×K	618.25	Joback Method
cpg	519.47	J/mol×K	655.56	Joback Method
cpg	538.03	J/mol×K	692.88	Joback Method

cpg	555.26	J/mol×K	730.19	Joback Method
cpg	571.16	J/mol×K	767.50	Joback Method
cpg	585.76	J/mol×K	804.82	Joback Method
cpg	599.07	J/mol×K	842.13	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=C953913&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

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