

Toluene-4-sulfonic acid, cyclohexyl ester

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,2-6H
InchiKey:	OHHPZPDQZMUTCA-UHFFFAOYSA-N
Formula:	C13H18O3S
SMILES:	<chem>Cc1ccc(S(=O)(=O)OC2CCCCC2)cc1</chem>
Mol. weight [g/mol]:	254.35

Physical Properties

Property code	Value	Unit	Source
hf	-515.72	kJ/mol	Cheméo Relay (1.0)
hfus	27.48	kJ/mol	Joback Method
hvap	91.98	kJ/mol	Cheméo Relay (1.0)
ie	8.71	eV	Cheméo Relay (1.0)
log10ws	-3.67		Cheméo Relay (1.0)
logp	3.033		Crippen Method
mcvol	193.370	ml/mol	McGowan Method
tb	624.62	K	Cheméo Relay (1.0)
tf	327.50	K	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C953913&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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