

2-Propyn-1-ol, 4-methylbenzenesulfonate

Other names:	p-Toluenesulfonic acid, 2-propynyl ester Propargyl p-toluene sulfonate 2-Propynyl p-Toluenesulfonate
Inchi:	InChI=1S/C10H10O3S/c1-3-8-13-14(11,12)10-6-4-9(2)5-7-10/h1,4-7H,8H2,2H3
InchiKey:	LMBVCSFXFFROTA-UHFFFAOYSA-N
Formula:	C10H10O3S
SMILES:	C#CCOS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	210.25
CAS:	6165-76-0

Physical Properties

Property code	Value	Unit	Source
gf	-214.37	kJ/mol	Joback Method
hf	-318.34	kJ/mol	Joback Method
hfus	30.85	kJ/mol	Joback Method
hvap	61.70	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.334		Crippen Method
mcvol	153.360	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	1666.00		NIST Webbook
rinpol	1666.00		NIST Webbook
tb	520.18	K	Joback Method
tc	732.17	K	Joback Method
tf	349.16	K	Joback Method
vc	0.594	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.69	J/mol×K	520.18	Joback Method
cpg	338.87	J/mol×K	555.51	Joback Method
cpg	351.32	J/mol×K	590.84	Joback Method
cpg	363.05	J/mol×K	626.17	Joback Method

cpg	374.07	J/mol×K	661.51	Joback Method
cpg	384.37	J/mol×K	696.84	Joback Method
cpg	393.96	J/mol×K	732.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6165760&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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