(P-TOLUENESULFONO)-P-TOLUIDE

Other names: N-(p-Toluene sulfonyl)-p-toluidide
N-(p-tolyl)-p-toluenesulphonamide
Inchi: InChI=1S/C14H15NO2S/c1-11-3-7-13(8-4-11)15-18(16,17)14-9-5-12(2)6-10-14/h3-10,15
InchiKey: GPLXRIVINNIQFY-UHFFFAOYSA-N
Formula: C14H15NO2S
SMILES: Cc1ccc(NS(=O)(=O)c2ccc(C)cc2)cc1
Mol. weight [g/mol]: 261.35

Physical Properties

Property code	Value	Unit	Source
hf	-175.06	kJ/mol	Cheméo Relay (1.0)
hfus	35.80	kJ/mol	Joback Method
hvap	101.67	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	-3.84		Cheméo Relay (1.0)
logp	3.104		Crippen Method
mcvol	198.670	ml/mol	McGowan Method
tb	649.61	K	Cheméo Relay (1.0)
tf	411.18	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.36	J/mol×K	680.99	Joback Method
cpg	525.04	J/mol×K	719.14	Joback Method
cpg	539.47	J/mol×K	757.29	Joback Method
cpg	552.70	J/mol×K	795.44	Joback Method
cpg	564.77	J/mol×K	833.60	Joback Method
cpg	575.70	J/mol×K	871.75	Joback Method
cpg	585.53	J/mol×K	909.90	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=C599860&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