o-(p-Toluylsulfonamido)aniline

Other names: p-Toluenesulfonamide, N-(o-aminophenyl)-
p-Toluenesulfonanilide, 2'-amino-
t-Sulfonamidine
Benzenesulfonamide, N-(2-aminophenyl)-4-methyl-
N 170
2-(p-Tolylsulfonylamino)aniline
2-(4-Toluenesulfonamido)aniline
o-(p-Toluylsulfonamido)aniline
2-(Tosylamino)aniline
NSC 116601
o-(p-Toluenesulfonamido)aniline

Inchi: InChI=1S/C13H14N2O2S/c1-10-6-8-11(9-7-10)18(16,17)15-13-5-3-2-4-12(13)14/h2-9,15

InchiKey: AQUNQTJQZYZXMR-UHFFFAOYSA-N

Formula: C13H14N2O2S

SMILES: Cc1ccc(S(=O)(=O)Nc2ccccc2N)cc1

Mol. weight [g/mol]: 262.33

Physical Properties

Property code	Value	Unit	Source
hf	-158.13	kJ/mol	Cheméo Relay (1.0)
hfus	38.40	kJ/mol	Joback Method
ie	7.41	eV	Cheméo Relay (1.0)
log10ws	-2.95		Cheméo Relay (1.0)
logp	2.378		Crippen Method
mcvol	194.560	ml/mol	McGowan Method
tf	440.20	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.24	J/mol×K	730.64	Joback Method
cpg	532.17	J/mol×K	770.44	Joback Method
cpg	544.83	J/mol×K	810.25	Joback Method
cpg	556.26	J/mol×K	850.05	Joback Method

cpg	566.50	J/mol×K	889.86	Joback Method
cpg	575.60	J/mol×K	929.66	Joback Method
cpg	583.58	J/mol×K	969.46	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3624906&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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