P-phenylenediamine, n,n-diethyl-n',n'-bis(p-tolylsulfonyl)-

InChI: InChI=1S/C24H28N2O4S2/c1-5-25(6-2)21-11-13-22(14-12-21)26(31(27,28)23-15-7-19(3)8-16-23)32(29,30)24-17-9-20(4)10-18-24/h7-18H,5-6H2,1-4H3

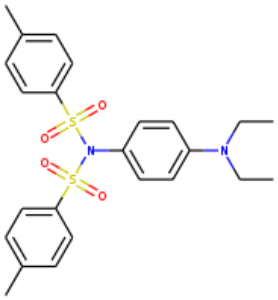
InChI Key: SZAOAPOETWBAFD-UHFFFAOYSA-N

Formula: C24H28N2O4S2

SMILES: CCN(CC)c1ccc(N(S(=O)(=O)c2ccc(C)cc2)S(=O)(=O)c2ccc(C)cc2)cc1

Molecular Weight: 472.62

CAS: 19770-88-8



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-255.98	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-635.15	kJ/mol	Joback Method
$\Delta_{fus} H°$	67.67	kJ/mol	Joback Method
$\Delta_{vap} H°$	119.19	kJ/mol	Joback Method
$logP_{oct/wat}$	4.73		Crippen Method
P_c	1944.08	kPa	Joback Method
T_{boil}	963.94	K	Joback Method
T_c	1191.77	K	Joback Method
T_{fus}	619.12	K	Joback Method
V_c	1.34	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1094.98	J/mol×K	963.94	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C24H28N2O4S2/c1-5-25(6-2)21-11-13-22(14-12-21)26(31(27,28)23-15-7-19(3)8-16-23)32(29,30)24-17-9-20(4)10-18-24/h7-18H,5-6H2,1-4H3

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).