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

InchiKey: SZAOAPOETWBAFD-UHFFFAOYSA-N

Formula: C24H28N2O4S2

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

Mol. weight [g/mol]: 472.62

CAS: 19770-88-8

Physical Properties

Property code	Value	Unit	Source
gf	-255.98	kJ/mol	Joback Method
hf	-635.15	kJ/mol	Joback Method
hfus	67.67	kJ/mol	Joback Method
hvap	119.19	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	4.734		Crippen Method
mcvol	353.880	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
tb	963.94	K	Joback Method
tc	1191.77	K	Joback Method
tf	619.12	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1094.98	J/mol×K	963.94	Joback Method
cpg	1107.94	J/mol×K	1001.91	Joback Method
cpg	1119.20	J/mol×K	1039.88	Joback Method
cpg	1128.82	J/mol×K	1077.85	Joback Method
cpg	1136.87	J/mol×K	1115.83	Joback Method
cpg	1143.44	J/mol×K	1153.80	Joback Method
cpg	1148.59	J/mol×K	1191.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19770888&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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