P-phenylenediamine, n,n-diethyl, n',n'-bis(3,4-dimethylphenyl sulfonyl)-

Inchi: InChI=1S/C26H32N2O4S2/c1-7-27(8-2)23-11-13-24(14-12-23)28(33(29,30)25-15-9-19(3

InchiKey: KLTGOXURDPDGLK-UHFFFAOYSA-N

Formula: C26H32N2O4S2

SMILES: CCN(CC)c1ccc(N(S(=O)(=O)c2ccc(C)c(C)c2)S(=O)(=O)c2ccc(C)c(C)c2)cc1

Mol. weight [g/mol]: 500.67

CAS: 19770-89-9

Physical Properties

Property code	Value	Unit	Source
gf	-258.40	kJ/mol	Joback Method
hf	-699.37	kJ/mol	Joback Method
hfus	72.07	kJ/mol	Joback Method
hvap	124.96	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.351		Crippen Method
mcvol	382.060	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
tb	1019.66	K	Joback Method
tc	1252.02	K	Joback Method
tf	666.70	K	Joback Method
vc	1.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1211.35	J/mol×K	1019.66	Joback Method
cpg	1223.55	J/mol×K	1058.39	Joback Method
cpg	1233.91	J/mol×K	1097.11	Joback Method
cpg	1242.50	J/mol×K	1135.84	Joback Method
cpg	1249.40	J/mol×K	1174.56	Joback Method
cpg	1254.66	J/mol×K	1213.29	Joback Method
cpg	1258.37	J/mol×K	1252.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19770899&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
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
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