P-phenylenediamine, n,n-diethyl-n',n'-bis(phenylsulfonyl)-

Inchi: InChI=1S/C22H24N2O4S2/c1-3-23(4-2)19-15-17-20(18-16-19)24(29(25,26)21-11-7-5-8-1

InchiKey: JUVRAEFALBENDT-UHFFFAOYSA-N

Formula: C22H24N2O4S2

SMILES: CCN(CC)c1ccc(N(S(=O)(=O)c2ccccc2)S(=O)(=O)c2ccccc2)cc1

Mol. weight [g/mol]: 444.57

CAS: 19770-87-7

Physical Properties

Property code	Value	Unit	Source
gf	-253.56	kJ/mol	Joback Method
hf	-570.93	kJ/mol	Joback Method
hfus	63.27	kJ/mol	Joback Method
hvap	113.41	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.117		Crippen Method
mcvol	325.700	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
tb	908.22	K	Joback Method
tc	1135.30	K	Joback Method
tf	571.54	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.02	J/mol×K	908.22	Joback Method
cpg	993.66	J/mol×K	946.07	Joback Method
cpg	1005.63	J/mol×K	983.91	Joback Method
cpg	1016.01	J/mol×K	1021.76	Joback Method
cpg	1024.89	J/mol×K	1059.60	Joback Method
cpg	1032.34	J/mol×K	1097.45	Joback Method
cpg	1038.45	J/mol×K	1135.30	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19770877&Units=SI

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

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