

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

Inchi:	InChI=1S/C20H20N2O4S2/c1-21(2)17-13-15-18(16-14-17)22(27(23,24)19-9-5-3-6-10-19
InchiKey:	FNNGNXVHDQDJJW-UHFFFAOYSA-N
Formula:	C20H20N2O4S2
SMILES:	CN(C)c1ccc(N(S(=O)(=O)c2ccccc2)S(=O)(=O)c2ccccc2)cc1
Mol. weight [g/mol]:	416.51
CAS:	19770-84-4

Physical Properties

Property code	Value	Unit	Source
gf	-270.40	kJ/mol	Joback Method
hf	-529.65	kJ/mol	Joback Method
hfus	58.09	kJ/mol	Joback Method
hvap	108.96	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.337		Crippen Method
mvol	297.520	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
tb	862.46	K	Joback Method
tc	1093.45	K	Joback Method
tf	549.00	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	864.80	J/molxK	862.46	Joback Method
cpg	878.76	J/molxK	900.96	Joback Method
cpg	891.01	J/molxK	939.46	Joback Method
cpg	901.66	J/molxK	977.96	Joback Method
cpg	910.76	J/molxK	1016.45	Joback Method
cpg	918.40	J/molxK	1054.95	Joback Method
cpg	924.65	J/molxK	1093.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19770844&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
mccvol:	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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