

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

Inchi:	InChI=1S/C24H28N2O4S2/c1-17-7-13-23(15-19(17)3)31(27,28)26(22-11-9-21(10-12-22)
InchiKey:	ZWXROISRYFYPME-UHFFFAOYSA-N
Formula:	C24H28N2O4S2
SMILES:	Cc1ccc(S(=O)(=O)N(c2ccc(N(C)C)cc2)S(=O)(=O)c2ccc(C)c(C)c2)cc1C
Mol. weight [g/mol]:	472.62
CAS:	19770-86-6

Physical Properties

Property code	Value	Unit	Source
gf	-275.24	kJ/mol	Joback Method
hf	-658.09	kJ/mol	Joback Method
hfus	66.89	kJ/mol	Joback Method
hvap	120.51	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	4.570		Crippen Method
mcvol	353.880	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
tb	973.90	K	Joback Method
tc	1203.40	K	Joback Method
tf	644.16	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.46	J/molxK	973.90	Joback Method
cpg	1105.06	J/molxK	1012.15	Joback Method
cpg	1115.89	J/molxK	1050.40	Joback Method
cpg	1125.01	J/molxK	1088.65	Joback Method
cpg	1132.48	J/molxK	1126.90	Joback Method
cpg	1138.37	J/molxK	1165.15	Joback Method
cpg	1142.72	J/molxK	1203.40	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=C19770866&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
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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