2-Methyl-1,4-di(phenylsulfonamido)naphthalene

Inchi: InChI=1S/C23H20N2O4S2/c1-17-16-22(24-30(26,27)18-10-4-2-5-11-18)20-14-8-9-15-21
InchiKey: LBDHRBVJFBGCHO-UHFFFAOYSA-N
Formula: C23H20N2O4S2
SMILES: Cc1cc(NS(=O)(=O)c2ccccc2)c2ccccc2c1NS(=O)(=O)c1ccccc1
Mol. weight [g/mol]: 452.55
CAS: 116401-66-2

Physical Properties

Property code	Value	Unit	Source
gf	-200.53	kJ/mol	Joback Method
hf	-451.56	kJ/mol	Joback Method
hfus	66.26	kJ/mol	Joback Method
hvap	127.39	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	4.750		Crippen Method
mcvol	320.330	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
tb	1035.50	K	Joback Method
tc	1285.19	K	Joback Method
tf	680.93	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.44	J/mol×K	1035.50	Joback Method
cpg	980.18	J/mol×K	1077.11	Joback Method
cpg	987.38	J/mol×K	1118.73	Joback Method
cpg	993.13	J/mol×K	1160.34	Joback Method
cpg	997.53	J/mol×K	1201.96	Joback Method
cpg	1000.71	J/mol×K	1243.57	Joback Method
cpg	1002.74	J/mol×K	1285.19	Joback Method

Sources

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=C116401662&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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