3-(4-Anilino-1-naphthylazo)-2,7-naphthalene disulfonic acid

Inchi: InChI=1S/C26H19N3O6S2/c30-36(31,32)20-11-10-17-15-25(26(37(33,34)35)16-18(17)14

InchiKey: BGHIEJHQLIHWPX-ZQHSETAFSA-N

Formula: C26H19N3O6S2

SMILES: O=S(=O)(O)c1ccc2cc(N=Nc3ccc(Nc4ccccc4)c4ccccc34)c(S(=O)(=O)O)cc2c1

Mol. weight [g/mol]: 533.58

CAS: 57322-42-6

Physical Properties

Property code	Value	Unit	Source
hf	-656.06	kJ/mol	Joback Method
hvap	170.62	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	6.645		Crippen Method
mcvol	360.560	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
tb	1416.47	K	Joback Method
tc	1756.26	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57322426&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

Legend

hf: Enthalpy of formation 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

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