N-benzoyl-4-nitro-3-phenylsulfonylaniline

Other names: Aniline, n-benzoyl-4-nitro-3-phenylsulfonyl-
Inchi: InChI=1S/C19H14N2O5S/c22-19(14-7-3-1-4-8-14)20-15-11-12-17(21(23)24)18(13-15)27
InchiKey: MZXKPYCBBLLYJM-UHFFFAOYSA-N
Formula: C19H14N2O5S
SMILES: O=[N+]([O-])c1ccc(N=C(O)c2ccccc2)cc1S(=O)(=O)c1ccccc1
Mol. weight [g/mol]: 382.39
CAS: 19770-93-5

Physical Properties

Property code	Value	Unit	Source
hf	-292.75	kJ/mol	Joback Method
hvap	121.34	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.064		Crippen Method
mcvol	264.350	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
tb	1092.48	K	Joback Method
tc	1357.21	K	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=C19770935&Units=SI

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