Aniline, n-benzoyl-4-nitro-3-phenylthio-

Inchi: InChI=1S/C19H14N2O3S/c22-19(14-7-3-1-4-8-14)20-15-11-12-17(21(23)24)18(13-15)25
InchiKey: BRKRZQIGOWNEEZ-UHFFFAOYSA-N
Formula: C19H14N2O3S
SMILES: O=[N+]([O-])c1ccc(N=C(O)c2ccccc2)cc1Sc1ccccc1
Mol. weight [g/mol]: 350.39
CAS: 19770-92-4

Physical Properties

Property code	Value	Unit	Source
hf	202.47	kJ/mol	Joback Method
hvap	109.52	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.382		Crippen Method
mcvol	252.610	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
tb	1113.48	K	Joback Method
tc	1395.51	K	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=C19770924&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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