Aniline, n,n-diethyl-4-nitro-3-phenylsulfonyl-

Inchi: InChI=1S/C16H18N2O4S/c1-3-17(4-2)13-10-11-15(18(19)20)16(12-13)23(21,22)14-8-6-5
InchiKey: KYINLEAHQCBTHL-UHFFFAOYSA-N
Formula: C16H18N2O4S
SMILES: CCN(CC)c1ccc([N+](=O)[O-])c(S(=O)(=O)c2ccccc2)c1
Mol. weight [g/mol]: 334.39
CAS: 19771-00-7

Physical Properties

Property code	Value	Unit	Source
gf	-32.81	kJ/mol	Joback Method
hf	-320.03	kJ/mol	Joback Method
hfus	50.26	kJ/mol	Joback Method
hvap	94.36	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.274		Crippen Method
mcvol	244.270	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
tb	840.86	K	Joback Method
tc	1078.42	K	Joback Method
tf	562.60	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.85	J/mol×K	840.86	Joback Method
cpg	722.38	J/mol×K	880.45	Joback Method
cpg	734.54	J/mol×K	920.05	Joback Method
cpg	745.38	J/mol×K	959.64	Joback Method
cpg	754.97	J/mol×K	999.24	Joback Method
cpg	763.38	J/mol×K	1038.83	Joback Method
cpg	770.67	J/mol×K	1078.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19771007&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

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