Benzamide, N-ethyl-N-[(4-ethylaminophenyl)sulfonyl]-

Inchi: InChI=1S/C17H20N2O3S/c1-3-18-15-10-12-16(13-11-15)23(21,22)19(4-2)17(20)14-8-6-5

InchiKey: NIDUGUJXKZMUFY-UHFFFAOYSA-N

Formula: C17H20N2O3S

SMILES: CCNc1ccc(S(=O)(=O)N(CC)C(=O)c2ccccc2)cc1

Mol. weight [g/mol]: 332.42

Physical Properties

Property code	Value	Unit	Source
gf	-89.84	kJ/mol	Joback Method
hf	-377.55	kJ/mol	Joback Method
hfus	48.58	kJ/mol	Joback Method
hvap	92.51	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	2.969		Crippen Method
mcvol	252.490	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	2116.00		NIST Webbook
rinpol	2116.00		NIST Webbook
tb	810.96	K	Joback Method
tc	1031.47	K	Joback Method
tf	520.33	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.81	J/mol×K	810.96	Joback Method
cpg	743.18	J/mol×K	847.71	Joback Method
cpg	756.24	J/mol×K	884.46	Joback Method
cpg	768.06	J/mol×K	921.22	Joback Method
cpg	778.68	J/mol×K	957.97	Joback Method
cpg	788.18	J/mol×K	994.72	Joback Method
cpg	796.60	J/mol×K	1031.47	Joback Method

Sources

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=U374448&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume