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

Inchi: InChI=1S/C15H16N2O3S/c1-2-17(15(18)12-6-4-3-5-7-12)21(19,20)14-10-8-13(16)9-11-1

InchiKey: URFQIOHQAZQIKQ-UHFFFAOYSA-N

Formula: C15H16N2O3S

SMILES: CCN(C(=O)c1ccccc1)S(=O)(=O)c1ccc(N)cc1

Mol. weight [g/mol]: 304.36

Physical Properties

Property code	Value	Unit	Source
gf	-129.62	kJ/mol	Joback Method
hf	-355.95	kJ/mol	Joback Method
hfus	43.49	kJ/mol	Joback Method
hvap	92.26	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.120		Crippen Method
mcvol	224.310	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook
tb	787.56	K	Joback Method
tc	1020.96	K	Joback Method
tf	528.39	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.89	J/mol×K	787.56	Joback Method
cpg	640.40	J/mol×K	826.46	Joback Method
cpg	652.59	J/mol×K	865.36	Joback Method
cpg	663.50	J/mol×K	904.26	Joback Method
cpg	673.21	J/mol×K	943.16	Joback Method
cpg	681.77	J/mol×K	982.06	Joback Method
cpg	689.24	J/mol×K	1020.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374447&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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