4-Ethylamino-N,N-diethylbenzenesulfamide

Inchi: InChI=1S/C12H20N2O2S/c1-4-13-11-7-9-12(10-8-11)17(15,16)14(5-2)6-3/h7-10,13H,4-6
InchiKey: XXXYSOMLDMCUMM-UHFFFAOYSA-N
Formula: C12H20N2O2S
SMILES: CCNc1ccc(S(=O)(=O)N(CC)CC)cc1
Mol. weight [g/mol]: 256.36

Physical Properties

Property code	Value	Unit	Source
gf	-115.43	kJ/mol	Joback Method
hf	-398.30	kJ/mol	Joback Method
hfus	39.99	kJ/mol	Joback Method
hvap	72.36	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.149		Crippen Method
mcvol	204.230	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
rinpol	1432.00		NIST Webbook
rinpol	1432.00		NIST Webbook
tb	616.01	K	Joback Method
tc	808.96	K	Joback Method
tf	387.63	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.01	J/mol×K	616.01	Joback Method
cpg	539.36	J/mol×K	648.17	Joback Method
cpg	554.76	J/mol×K	680.33	Joback Method
cpg	569.23	J/mol×K	712.48	Joback Method
cpg	582.79	J/mol×K	744.64	Joback Method
cpg	595.47	J/mol×K	776.80	Joback Method
cpg	607.29	J/mol×K	808.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374768&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
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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