Nl,nl-diethylsulfanilamide

Other names: 4-amino-N,N-diethylbenzenesulfonamide
N
Inchi: InChI=1S/C10H16N2O2S/c1-3-12(4-2)15(13,14)10-7-5-9(11)6-8-10/h5-8H,3-4,11H2,1-2H
InchiKey: LTFVELCIFWEGGA-UHFFFAOYSA-N
Formula: C10H16N2O2S
SMILES: CCN(CC)S(=O)(=O)c1ccc(N)cc1
Mol. weight [g/mol]: 228.32

Physical Properties

Property code	Value	Unit	Source
hfus	34.90	kJ/mol	Joback Method
ie	7.29	eV	Cheméo Relay (1.0)
log10ws	-2.65		Cheméo Relay (1.0)
logp	1.299		Crippen Method
mcvol	176.050	ml/mol	McGowan Method
tb	640.37	K	Cheméo Relay (1.0)
tf	378.80	K	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.11	J/mol×K	592.61	Joback Method
cpg	449.16	J/mol×K	626.94	Joback Method
cpg	463.27	J/mol×K	661.27	Joback Method
cpg	476.46	J/mol×K	695.61	Joback Method
cpg	488.76	J/mol×K	729.94	Joback Method
cpg	500.18	J/mol×K	764.27	Joback Method
cpg	510.76	J/mol×K	798.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1709393&Units=SI
Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents:	https://www.doi.org/10.1021/je500918t
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0, beta):	
Octanol/Water Partition Coefficients of Sulfonamides: Experimental Determination and Calculation Using Physicochemical Descriptors:	https://www.doi.org/10.1021/je900189v

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point