Tetraethyl sulphamide

Other names: N,N,N',N'-Tetraethylsulfamide
N-(diethylsulfamoyl)-N-ethylethanamine
Inchi: InChI=1S/C8H20N2O2S/c1-5-9(6-2)13(11,12)10(7-3)8-4/h5-8H2,1-4H3
InchiKey: IYIAWAACGTUPCC-UHFFFAOYSA-N
Formula: C8H20N2O2S
SMILES: CCN(CC)S(=O)(=O)N(CC)CC
Mol. weight [g/mol]: 208.32
CAS: 2832-49-7

Physical Properties

Property code	Value	Unit	Source
gf	-230.50	kJ/mol	Joback Method
hf	-526.74	kJ/mol	Joback Method
hfl	-635.50 ± 9.90	kJ/mol	NIST Webbook
hfus	33.90	kJ/mol	Joback Method
hvap	56.12	kJ/mol	Joback Method
log10ws	-1.14		Aqueous Solubility Prediction Method
logp	0.915		Crippen Method
mcvol	171.630	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
tb	455.10	K	Joback Method
tc	614.57	K	Joback Method
tf	283.42	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.10	J/mol×K	587.99	Joback Method
cpg	373.92	J/mol×K	455.10	Joback Method
cpg	389.16	J/mol×K	481.68	Joback Method
cpg	403.79	J/mol×K	508.26	Joback Method
cpg	417.81	J/mol×K	534.83	Joback Method

cpg	431.25	J/mol×K	561.41	Joback Method
cpg	456.39	J/mol×K	614.57	Joback Method
hvapt	59.10	kJ/mol	467.50	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2832497&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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