1-(([(Diethylamino)carbonyl]amino)sulfonyl)-4-me

Inchi: InChI=1S/C12H18N2O3S/c1-4-14(5-2)12(15)13-18(16,17)11-8-6-10(3)7-9-11/h6-9H,4-5H
InchiKey: QZJMCHATEVRINW-UHFFFAOYSA-N
Formula: C12H18N2O3S
SMILES: CCN(CC)C(=O)NS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 270.35
CAS: 23730-10-1

Physical Properties

Property code	Value	Unit	Source
gf	-244.35	kJ/mol	Joback Method
hf	-510.88	kJ/mol	Joback Method
hfus	41.58	kJ/mol	Joback Method
hvap	79.10	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.735		Crippen Method
mcvol	205.800	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
tb	669.88	K	Joback Method
tc	869.85	K	Joback Method
tf	437.56	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.14	J/mol×K	669.88	Joback Method
cpg	558.92	J/mol×K	703.21	Joback Method
cpg	572.73	J/mol×K	736.54	Joback Method
cpg	585.57	J/mol×K	769.87	Joback Method
cpg	597.48	J/mol×K	803.20	Joback Method
cpg	608.48	J/mol×K	836.52	Joback Method
cpg	618.59	J/mol×K	869.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23730101&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume