N-(2-Methoxypropionyl)-4,N-dimethyl-benzenesul

Inchi: InChI=1S/C12H17NO4S/c1-9-5-7-11(8-6-9)18(15,16)13(3)12(14)10(2)17-4/h5-8,10H,1-4
InchiKey: GWAXTTJRMWNOGT-UHFFFAOYSA-N
Formula: C12H17NO4S
SMILES: COC(C)C(=O)N(C)S(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 271.33

Physical Properties

Property code	Value	Unit	Source
gf	-441.18	kJ/mol	Joback Method
hf	-701.85	kJ/mol	Joback Method
hfus	34.15	kJ/mol	Joback Method
hvap	74.69	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.177		Crippen Method
mcvol	201.690	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	1980.00		NIST Webbook
rinpol	1980.00		NIST Webbook
tb	641.69	K	Joback Method
tc	843.15	K	Joback Method
tf	392.13	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.24	J/mol×K	641.69	Joback Method
cpg	532.54	J/mol×K	675.27	Joback Method
cpg	546.89	J/mol×K	708.84	Joback Method
cpg	560.27	J/mol×K	742.42	Joback Method
cpg	572.71	J/mol×K	776.00	Joback Method
cpg	584.21	J/mol×K	809.57	Joback Method
cpg	594.79	J/mol×K	843.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374399&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