1,4-Dimethoxy-2-(methylthio)-benzene

Inchi: InChI=1S/C9H12O2S/c1-10-7-4-5-8(11-2)9(6-7)12-3/h4-6H,1-3H3
InchiKey: VDHGQPCJOZRMTC-UHFFFAOYSA-N
Formula: C9H12O2S
SMILES: COc1ccc(OC)c(SC)c1
Mol. weight [g/mol]: 184.25
CAS: 2570-42-5

Physical Properties

Property code	Value	Unit	Source
gf	-58.83	kJ/mol	Joback Method
hf	-238.07	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	50.86	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.426		Crippen Method
mcvol	142.000	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
ripol	2334.00		NIST Webbook
tb	555.58	K	Joback Method
tc	782.79	K	Joback Method
tf	321.51	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.54	J/mol×K	555.58	Joback Method
cpg	324.72	J/mol×K	593.45	Joback Method
cpg	337.29	J/mol×K	631.32	Joback Method
cpg	349.20	J/mol×K	669.18	Joback Method
cpg	360.45	J/mol×K	707.05	Joback Method
cpg	371.02	J/mol×K	744.92	Joback Method
cpg	380.87	J/mol×K	782.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2570425&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume