2,5-Dimethoxythiophenol

Inchi: InChI=1S/C8H10O2S/c1-9-6-3-4-7(10-2)8(11)5-6/h3-5,11H,1-2H3
InchiKey: SESUUAOAUZDHHP-UHFFFAOYSA-N
Formula: C8H10O2S
SMILES: COc1ccc(OC)c(S)c1
Mol. weight [g/mol]: 170.23
CAS: 1483-27-8

Physical Properties

Property code	Value	Unit	Source
gf	-70.98	kJ/mol	Joback Method
hf	-220.82	kJ/mol	Joback Method
hfus	16.16	kJ/mol	Joback Method
hvap	48.56	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	1.992		Crippen Method
mcvol	127.910	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	526.78	K	Joback Method
tc	758.79	K	Joback Method
tf	312.30	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.42	J/mol×K	526.78	Joback Method
cpg	277.34	J/mol×K	565.45	Joback Method
cpg	288.71	J/mol×K	604.12	Joback Method
cpg	299.51	J/mol×K	642.79	Joback Method
cpg	309.73	J/mol×K	681.45	Joback Method
cpg	319.36	J/mol×K	720.12	Joback Method
cpg	328.37	J/mol×K	758.79	Joback Method

Sources

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=C1483278&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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