5,5'-Thiodisalicylic acid, dimethyl ester

Other names: Thio bis-(5,5'-salicylic acid, dimethyl ester)
Inchi: InChI=1S/C16H14O6S/c1-21-15(19)11-7-9(3-5-13(11)17)23-10-4-6-14(18)12(8-10)16(20
InchiKey: KVTWYSPFORFKDI-UHFFFAOYSA-N
Formula: C16H14O6S
SMILES: COC(=O)c1cc(Sc2ccc(O)c(C(=O)OC)c2)ccc1O
Mol. weight [g/mol]: 334.34
CAS: 24483-72-5

Physical Properties

Property code	Value	Unit	Source
gf	-454.56	kJ/mol	Joback Method
hf	-725.80	kJ/mol	Joback Method
hfus	45.77	kJ/mol	Joback Method
hvap	108.24	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.822		Crippen Method
mcvol	231.750	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
tb	1011.40	K	Joback Method
tc	1273.22	K	Joback Method
tf	750.12	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.14	J/mol×K	1011.40	Joback Method
cpg	702.47	J/mol×K	1055.04	Joback Method
cpg	713.55	J/mol×K	1098.67	Joback Method
cpg	724.52	J/mol×K	1142.31	Joback Method
cpg	735.53	J/mol×K	1185.94	Joback Method
cpg	746.73	J/mol×K	1229.58	Joback Method
cpg	758.25	J/mol×K	1273.22	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=C24483725&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