[4-(4-Trifluoroacetoxy-5-tert-butyl-2-methylphenyl trifluoroacetate

Other names: 4,4'-Thiobis(2-tert-butyl-1-hydroxy-5-methylphenyl), bistrifluoroacetate
Thiobis-2-tert-butyl-5-methyl-4,1-phenylene bis(trifluoroacetate)

Inchi: InChI=1S/C26H28F6O4S/c1-13-9-17(35-21(33)25(27,28)29)15(23(3,4)5)11-19(13)37-20-

InchiKey: IDGHOYVDCDSOQP-UHFFFAOYSA-N

Formula: C26H28F6O4S

SMILES: Cc1cc(OC(=O)C(F)(F)F)c(C(C)(C)C)cc1Sc1cc(C(C)(C)C)c(OC(=O)C(F)(F)F)cc1C

Mol. weight [g/mol]: 550.55

Physical Properties

Property code	Value	Unit	Source
gf	-1257.14	kJ/mol	Joback Method
hf	-1835.12	kJ/mol	Joback Method
hfus	47.37	kJ/mol	Joback Method
hvap	97.04	kJ/mol	Joback Method
log10ws	-9.42		Crippen Method
logp	7.985		Crippen Method
mcvol	371.530	ml/mol	McGowan Method
pc	960.29	kPa	Joback Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
tb	1081.58	K	Joback Method
tc	1324.25	K	Joback Method
tf	702.68	K	Joback Method
vc	1.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1222.68	J/mol×K	1081.58	Joback Method
cpg	1234.44	J/mol×K	1122.03	Joback Method
cpg	1245.20	J/mol×K	1162.47	Joback Method
cpg	1255.11	J/mol×K	1202.92	Joback Method
cpg	1264.31	J/mol×K	1243.36	Joback Method
cpg	1272.94	J/mol×K	1283.81	Joback Method

cpg	1281.15	J/mol×K	1324.25	Joback Method

Sources

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=U373408&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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