4-tert-Butylcatechol, bis(trifluoroacetate)

Other names: Pyrocatechol, 5-tert.-butyl, bis-TFA
Inchi: InChI=1S/C14H12F6O4/c1-12(2,3)7-4-5-8(23-10(21)13(15,16)17)9(6-7)24-11(22)14(18,1
InchiKey: CGEZWQNDCPALEZ-UHFFFAOYSA-N
Formula: C14H12F6O4
SMILES: CC(C)(C)c1ccc(OC(=O)C(F)(F)F)c(OC(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 358.23

Physical Properties

Property code	Value	Unit	Source
gf	-1468.03	kJ/mol	Joback Method
hf	-1811.21	kJ/mol	Joback Method
hfus	27.09	kJ/mol	Joback Method
hvap	59.88	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.919		Crippen Method
mcvol	209.860	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
tb	694.87	K	Joback Method
tc	884.41	K	Joback Method
tf	454.12	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.84	J/mol×K	694.87	Joback Method
cpg	606.80	J/mol×K	726.46	Joback Method
cpg	617.89	J/mol×K	758.05	Joback Method
cpg	628.14	J/mol×K	789.64	Joback Method
cpg	637.62	J/mol×K	821.23	Joback Method
cpg	646.37	J/mol×K	852.82	Joback Method
cpg	654.43	J/mol×K	884.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U365441&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