2-Hydroxyphenol bis(trifluoroactate)

Other names:	2-[(2,2,2-Trifluoroacetyl)oxy]phenyl trifluoroacetate
	2-Hydroxyphenol di-TFA
	Acetic acid, trifluoro-, O-phenylene ester
	O-Phenylene trifluoroacetate
	Pyrocatechol, bis-TFA
Inchi:	InChI=1S/C10H4F6O4/c11-9(12,13)7(17)19-5-3-1-2-4-6(5)20-8(18)10(14,15)16/h1-4H
InchiKey:	HCNDLYNWFQKHJZ-UHFFFAOYSA-N
Formula:	C10H4F6O4
SMILES:	O=C(Oc1ccccc1OC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]:	302.13
CAS:	23529-06-8

Physical Properties

Property code	Value	Unit	Source
gf	-1494.92	kJ/mol	Joback Method
hf	-1708.43	kJ/mol	Joback Method
hfus	24.53	kJ/mol	Joback Method
hvap	51.61	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.622		Crippen Method
mcvol	153.500	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
tb	601.60	K	Joback Method
tc	788.25	K	Joback Method
tf	394.10	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.32	J/mol×K	601.60	Joback Method
cpg	405.05	J/mol×K	632.71	Joback Method

cpg	414.07	J/mol×K	663.82	Joback Method
cpg	422.42	J/mol×K	694.92	Joback Method
cpg	430.10	J/mol×K	726.03	Joback Method
cpg	437.17	J/mol×K	757.14	Joback Method
cpg	443.64	J/mol×K	788.25	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=C23529068&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume