4-HYDROXYPHENOL DITFA

Other names: 4-[(2,2,2-Trifluoroacetyl)oxy]phenyl trifluoroacetate
4-Hydroxyphenol, di-TFA
Hydroquinone, bis-trifluoroacetate
Inchi: InChI=1S/C10H4F6O4/c11-9(12,13)7(17)19-5-1-2-6(4-3-5)20-8(18)10(14,15)16/h1-4H
InchiKey: JNIQQHFSXLXIMY-UHFFFAOYSA-N
Formula: C10H4F6O4
SMILES: O=C(Oc1ccc(OC(=O)C(F)(F)F)cc1)C(F)(F)F
Mol. weight [g/mol]: 302.13

Physical Properties

Property code	Value	Unit	Source
hf	-1805.23	kJ/mol	Cheméo Relay (1.0)
hfus	24.53	kJ/mol	Joback Method
hvap	68.89	kJ/mol	Cheméo Relay (1.0)
ie	9.52	eV	Cheméo Relay (1.0)
logp	2.622		Crippen Method
mcvol	153.500	ml/mol	McGowan Method
rinpol	1030.00		NIST Webbook
rinpol	1030.00		NIST Webbook
tb	464.37	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34065731&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature