Pyrocatechol, 4-tert.-butyl, TFA-PFP

Inchi: InChI=1S/C15H12F8O4/c1-12(2,3)7-4-5-8(26-11(25)14(18,19)20)9(6-7)27-10(24)13(16,1
InchiKey: GZQGVFISYTVXCI-UHFFFAOYSA-N
Formula: C15H12F8O4
SMILES: CC(C)(C)c1ccc(OC(=O)C(F)(F)F)c(OC(=O)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 408.24

Physical Properties

Property code	Value	Unit	Source
gf	-1846.39	kJ/mol	Joback Method
hf	-2232.82	kJ/mol	Joback Method
hfus	28.43	kJ/mol	Joback Method
hvap	59.18	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.555		Crippen Method
mcvol	227.490	ml/mol	McGowan Method
pc	1539.08	kPa	Joback Method
rinpol	1286.00		NIST Webbook
rinpol	1286.00		NIST Webbook
tb	713.06	K	Joback Method
tc	896.87	K	Joback Method
tf	468.99	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.67	J/mol×K	713.06	Joback Method
cpg	677.34	J/mol×K	743.70	Joback Method
cpg	688.13	J/mol×K	774.33	Joback Method
cpg	698.10	J/mol×K	804.97	Joback Method
cpg	707.29	J/mol×K	835.60	Joback Method
cpg	715.78	J/mol×K	866.24	Joback Method
cpg	723.63	J/mol×K	896.87	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=R335550&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