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

Inchi: InChI=1S/C16H12F10O4/c1-12(2,3)7-4-5-8(29-11(28)14(19,20)21)9(6-7)30-10(27)13(17
InchiKey: KBHIFEMJPTXRFM-UHFFFAOYSA-N
Formula: C16H12F10O4
SMILES: CC(C)(C)c1ccc(OC(=O)C(F)(F)F)c(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 458.25

Physical Properties

Property code	Value	Unit	Source
gf	-2224.75	kJ/mol	Joback Method
hf	-2654.43	kJ/mol	Joback Method
hfus	29.76	kJ/mol	Joback Method
hvap	58.47	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.190		Crippen Method
mcvol	245.120	ml/mol	McGowan Method
pc	1355.63	kPa	Joback Method
rinpol	1332.00		NIST Webbook
rinpol	1332.00		NIST Webbook
tb	731.25	K	Joback Method
tc	910.94	K	Joback Method
tf	483.86	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.88	J/mol×K	731.25	Joback Method
cpg	748.28	J/mol×K	761.20	Joback Method
cpg	758.79	J/mol×K	791.15	Joback Method
cpg	768.48	J/mol×K	821.10	Joback Method
cpg	777.42	J/mol×K	851.04	Joback Method
cpg	785.69	J/mol×K	880.99	Joback Method
cpg	793.35	J/mol×K	910.94	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=R335545&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