4-tert-Butylcatechol, O,O'-bis(heptafluorobutyrate)

Other names: Pyrocatechol, 4-tert.-butyl, bis-HFB
Inchi: InChI=1S/C18H12F14O4/c1-12(2,3)7-4-5-8(35-10(33)13(19,20)15(23,24)17(27,28)29)9(6
InchiKey: BUKUNDXYDAVYCJ-UHFFFAOYSA-N
Formula: C18H12F14O4
SMILES: CC(C)(C)c1ccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 558.26

Physical Properties

Property code	Value	Unit	Source
gf	-2981.47	kJ/mol	Joback Method
hf	-3497.65	kJ/mol	Joback Method
hfus	32.43	kJ/mol	Joback Method
hvap	57.06	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.461		Crippen Method
mcvol	280.380	ml/mol	McGowan Method
pc	1074.98	kPa	Joback Method
rinpol	1399.00		NIST Webbook
tb	767.63	K	Joback Method
tc	944.07	K	Joback Method
tf	513.60	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.14	J/mol×K	767.63	Joback Method
cpg	891.08	J/mol×K	797.04	Joback Method
cpg	901.15	J/mol×K	826.44	Joback Method
cpg	910.42	J/mol×K	855.85	Joback Method
cpg	919.00	J/mol×K	885.25	Joback Method
cpg	926.98	J/mol×K	914.66	Joback Method
cpg	934.46	J/mol×K	944.07	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U365295&Units=SI

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